TRANS-BOUNDARY POLLUTANT IMPACTS OF EMISSIONS IN THE IMPERIAL VALLEY-CALEXICO REGION AND FROM SOUTHERN CALIFORNIA

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Santosh Chandru

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TRANSBOUNDARY POLLUTANT IMPACTS OF EMISSIONS IN THE IMPERIAL VALLEY-CALEXICO REGION AND FROM SOUTHERN CALIFORNIA

Approved by:

Dr. Armistead G. Russell, Advisor
School of Civil and Environmental Engineering
Georgia Institute of Technology

Dr. Talat Odman
School of Civil and Environmental Engineering
Georgia Institute of Technology

Dr. James Mulholland
School of Civil and Environmental Engineering
Georgia Institute of Technology

Date Approved: May 12, 2008

To my family

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LIST OF SYMBOLS AND ABBREVIATIONS

USEPA	United States Environmental Protection Agency
CMAQ	Community Multiscale Air Quality model
MCIP	Meteorology Chemistry Interface Processor
SMOKE	Sparse Matrix Operator and Kernel Emissions
MIMS	Multimedia Integrated Management System
MM5	Fifth Generation Mesoscale Meteorological Model
PAVE	Package for Analysis and Visualization of Environmental data
AQM	Air Quality Model
CCTM	CMAQ Chemical Transport Model
NEI	National Emission Inventory
SAPRC	Statewide Air Pollution Research Center
CAMS	Continuous Air Monitoring Stations
CART	Classification and Regression Tree
SCC	Source Classification Code
VMT	Vehicle Miles Travelled
DOE	Department of Energy
TPT	Third Party Testing
CAREG	California Regulations
TAF	Tracking and Analysis Framework
COI	Cost of Illness
WTP	Willingness to Pay

SEMARNAT	Secretaría de Medio Ambiente y Recursos Naturales
ISESALUD	Instituto de Servicios de Salud Pública del Estado de Baja California
UABC	Universidad Autónoma de Baja California
CARB	California Air Resources Board
CMB	Chemical Mass Balance
MOHAVE	Measurement of Haze and Visual Effects

CHAPTER 1

INTRODUCTION

1.1 Overview

Trans-boundary air pollution across United States and Mexico is a rising problem due to increased commercial and industrial activities in the border regions. Current air quality in Mexico indicate that urban centers like Mexico City, Monterrey, Guadalajara, Toluca, Ciudad Juarez, Mexicali and Tijuana continue to exceed the Mexican Air Quality Standards for ozone (O_3) and particulate matter less than 10 µm in diameter (PM_{10}), while other cities are starting to show warning signs of future air quality problems [1]. The World Bank estimates that the costs associated with environmental degradation represent nearly 10% of Mexico's Gross Domestic Product [2], while energy depletion accounts for 4% [3]. The western part of the border between Mexico and the United States consists of two primary regions (Figure 1.1), Tijuana-San Diego and Mexicali-Calexico (Imperial Valley). Tijuana-San Diego has been a border economical belt for a long time. Over the last fifteen years Mexicali has been one of the fastest-growing cities in Mexico in terms of industrial development, job creation, and energy demand. The resulting increase in air pollution and environmental degradation presents challenges as well as opportunities for achieving sustainable and socially responsible economic growth.

A report on air quality in Mexicali issued by the Secretaría de Medio Ambiente y Recursos Naturales (SEMARNAT), the Mexican environmental agency, states that ozone-causing pollutants and fine suspended particulate matter have reached critical levels. Similar reports from the U.S. Environmental Protection Agency and the State of California confirm this data [4].

Figure 1.1 Map representing the regions of Mexicali-Calexico and Tijuana-San Diego

Harmful contaminants in the border region originate from a number of sources, including motor vehicles, unpaved roads, farms, power plants, and factories. Geothermal power plants, light manufacturing operations, waste disposal sites, mining, and aggregate handling are also located near the border. Mexicali and the Imperial Valley have similar environmental regulations for carbon monoxide (CO), O_3, and PM_{10}, and both regions are non-compliant with air quality standards. Imperial Valley has also been designated by USEPA as non-attainment for O_3 for many years now (Figure 1.2). In Mexicali–Calexico poorly maintained vehicles contribute to the levels of carbon monoxides, nitrogen oxides, and hydrocarbons in the air. Mexicali, with a population of around 870,000 consists of 45% vehicles that are older than 1980, 48% are models from 1981 to 1990, and the remaining models from or after 1991. Burning of trash, tires, and other materials are also the sources of PM, sulfur dioxides, and carbon monoxide. Driving on unpaved roads, illegal dumping, and other common behaviors of individuals are additional contributors to PM.

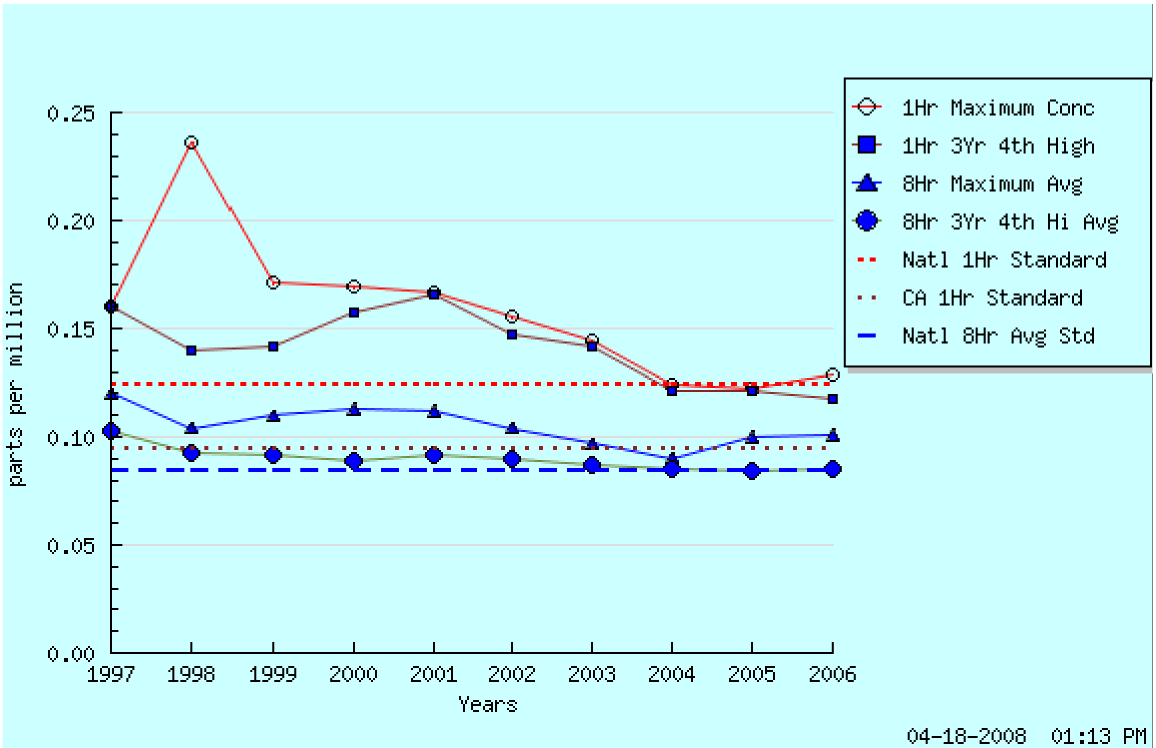

Figure 1.2 Ozone concentration trend from 1997 to 2006 in Imperial Valley
Source: California Air Resources Board (CARB), 2006

The resulting air pollution has thus been linked to high rates of asthma and respiratory diseases on both sides of the border [5]. Instituto de Servicios de Salud Pública del Estado de Baja California (ISESALUD) reports that the number of patients (primarily children and elderly) hospitalized for respiratory infections in the region is increasing. Studies conducted by the Environmental Studies Department at UABC have also shown that O_3, CO, and PM_{10} are the primary pollutants that have a direct or indirect consequence on the patients studied.

1.2 Previous Studies

Several studies have been conducted in the past 15 years in order to understand the composition, spatial variability, and sources of air pollution in the Mexicali-Calexico region.

As part of the 1983 US-Mexico Border Environmental Agreement (La Paz Agreement), a three-year effort from 1991 to 1994, a study was conducted to understand the effects of cross-border transport on suspended particles in the Imperial Valley-Mexicali region [6, 7]. The potential sources of PM_{10} in Imperial Valley were identified as: Fugitive dust (e.g., paved/unpaved road dust, windblown dust, agricultural tilling, construction, aggregate mining/handling, from the Salton Sea), motor vehicle exhaust (e.g., on-road/off-road vehicles, farm implements), field burning (e.g., asparagus and wheat crops), secondary aerosol formation, and pollution transport from Los Angeles, Palm Springs, and Mexicali. Due to the lack of monitoring sites in Mexicali, meteorological data was sparse. On average, when the wind was blowing from Mexico (i.e., southerly flow), the PM_{10} flux at Calexico was three times greater than when the wind was blowing from the United States (i.e., northerly flow). However, because transport from the north was about twice as frequent as transport from the south, the total flux from Mexico was only about one-and-one-half times the total flux from the United States. PM_{10} mass concentrations at the Mexicali site were consistently 30% to 50% higher than those observed at the Calexico site. Crustal material was the most abundant component and accounted for 50% to 62% of PM_{10} mass. Carbon was the second most abundant component, accounting for over 25% of PM_{10} mass. Further, a Chemical Mass Balance (CMB) method was also applied to the data, and results showed that the relative source mix at the pollutant monitoring sites in Mexicali and Calexico were similar, even though the absolute PM_{10} mass concentrations and source contributions were approximately twice as high at the Mexicali site. It also showed that geological material, motor vehicle exhaust, and vegetative burning source contributions were largest during the winter. Marine aerosol contributions were largest during the summer and spring; and uniformly low during the winter. Air quality trends in the US-Mexico border regions [8] again reiterated the air pollution problem in Mexicali-Calexico caused from anthropogenic sources such as motor vehicles, industrial activities, and also from soil dust and agricultural activities in the region. Trends also indicated higher O_3 levels in Mexicali on days of higher border crossing traffic.

Project MOHAVE was a major project to investigate the causes of visibility impairment to the Grand Canyon National Park region. The primary aim was determine the air quality deterioration caused from the Mohave Power plant. Analysis of the data collected during the project found that, one of the monitoring sites, ‘Meadview’, which was located west of the national park, showed three times SO_2 concentrations than the peak observed in the past six years [9]. Investigating the data made it clear that the contribution from the Mohave Power plant was close to the expected levels, hence other source contributions resulting to the tripling of the SO_2 concentrations had to be investigated. CMB analysis of the data gave estimates of the source contribution from regions such as South Coast Air Basin, Baja California, Arizona, and San Joaquin Valley. The source profiles showed transport of pollutants from Mexico and the Imperial Valley up the Colorado River Valley during the summer. The profiles also represented the contribution from larger point sources, apart from small but many SO_2 sources in the Mexicali-Calexico border region.

Apart from measures to characterize the sources, and concentrations of pollutants, strategic studies were also conducted in order to analyze the growth of the Mexicali-Calexico border, and also to predict the impact on air quality due to growth in energy demand. In a study to assess the environmental impacts of the current and proposed power plants in California-Baja California border region the most significant realization and conclusion is that the current level of air pollution emissions due to power production could be dramatically reduced by replacing existing base-load power plant technology with modern power plant equipment and technology, and also by using innovative methods to meet the 2030 power demand. The basis of this conclusion is that the existing base-load power plants in 2001 were emitting more than eight times CO and more than four times NOx than what an equivalent-sized combined cycle power plant would emit. Therefore, the regional supply of power could be approximately doubled while per-year reductions of 76% for CO emissions and 64% for NOx emissions are realized [10].

1.3 Scope of this work

1.3.1 Objective 1

As mentioned in section 1.2, studies to understand source contributions and concentrations of PM_{10} have been conducted over the lower California areas. These studies were limited to analyzing PM_{10} dynamics and the need to study the dynamics of particulate matter less than 2.5 μm ($PM_{2.5}$) and O_3 over the region still remains. Long range transport of various pollutants is important in regional air quality assessments. Though, there have been projects to monitor and assess pollutant concentration levels in Tijuana, San Diego, Mexicali and Calexico individually, a combined effort to understand the pollutant interaction and transport between these border regions was lacking.

Objective 1 of this thesis presented in Chapter 3 focuses on pollutant formation and pollutant interactions between the three regions of the Mexicali-Imperial Valley, Tijuana-San Diego, and Los Angeles areas. The one-atmosphere Community Multiscale Air Quality (CMAQ) modeling approach [11] is used for analyzing the formation of secondary species, and transport of both primary and secondary pollutants between the above mentioned regions during three pollution episodes in July 2001, August 2001, and January 2002. Impacts of particular sources/source contribution from within the region and from other regions during summer and winter episodes is conducted using the sensitivity analysis approach with CMAQ/ Decoupled Direct Method (DDM) [12, 13].

1.3.2 Objective 2

Future energy requirement studies have been able to project pollutant emissions from the growing number of power plants in the border regions; however the transport of pollutants and their impacts on either sides of the border has not been conducted. Concerns have increased over the impact of power plant emissions that are being commissioned in the border regions which supply energy to the growing needs in the border region and parts of California. Two such natural gas-fired combined-cycle power plants, La Rosarita Power Complex (LRPC) and Termoeléctrica de Mexicali (TDM) (henceforth commonly addressed as Intergen and Sempra in this thesis) located in Mexicali, 7 miles away from the US-Mexico border are studied. (LRPC has two separate units. LR-1 (unit 1) is partly owned and operated Energia Azteca X S. de R.L. de C.V. (EAX), a subsidiary of InterGen power company having a capacity of 750 MW of which 660 MW are contracted by CFE (Comisión Federal de Electricidad, the government enterprise tasked with the ownership and operation of the public electric system infrastructure) under a power purchase agreement and 90 MW are exported to California. LR-2 (unit 2) owned by Energia de Baja California (EBC) S. de R.L. de C.V. has a capacity of 310 MW exclusively dedicated to export. TDM, a Sempra subsidiary owns and operates the 650 MW combined cycle generating facility located very close to Intergen. The power plant produces electricity exclusively for export to the United States, transmitted over a transmission line not connected to the CFE transmission system.

In Chapter 4, air quality modeling simulations using CMAQ/DDM3D-PM [14] are performed to estimate the impact of Intergen and Sempra emissions on concentration levels of pollutants in the region during a summer pollution episode in 2001, and a winter pollution episode in 2002. PM from unpaved roads being a primary area of concern, additional results are analyzed on a scenario in which all the roads in Mexicali are paved. This will help in analyzing the air quality benefits of paving roads in the border region. The Tracking and Analysis Framework (TAF) model [15] is used to estimate preliminary health impacts from O_3 and $PM_{2.5}$ contribution from these power plants on the regions of Baja California, Sonora, California, Nevada, and Arizona. The health impact work using the TAF model is being conducted by Dr. Allen Blackman and Zhuxuan You at Resources for the Future (RFF), Washington DC. The health impact work being in progress, the discussion is Chapter 4 is confined to the air quality impacts from the two power plants on O_3 and $PM_{2.5}$ concentrations in the border region.

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CHAPTER 2

MODELING APPROACH

2.1 Overview

The one-atmosphere Community Multi-scale Air Quality (CMAQ) [1] model which has the state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric O_3, fine particles, toxics, acid deposition, and visibility reduction has been used to simulate the episodes. Input preparation for CMAQ starts by selecting the representative pollution episodes during the particular years. Episode selection during the years 2001 and 2002 was performed using the Classification and Regression Trees (CART) analysis. The Fifth generation Mesoscale Meteorological Model (MM5) is then used to simulate the Meteorological fields during the episodes. In order to use the meteorological outputs from MM5, they are converted to model ready format using the Meteorology Chemistry Interface Processor (MCIP). Gridded emissions from various primary sources are prepared using the Sparse Matrix Operator Kernel for Emissions (SMOKE). Outputs of MCIP and SMOKE form the primary inputs to CMAQ. Source contribution from various sources is simulated using the CMAQ/ Decoupled Direct Method. In order to find the health impacts from O_3 and $PM_{2.5}$ concentrations on the border region, the output from CMAQ/DDM forms one of the inputs for the Tracking and Analysis Framework (TAF) model. The modeling approach used for this thesis is represented in Figure 2.1.

2.2 Episode Selection

Selection of modeling episodes constitutes a fundamental part of the modeling process. Emissions along with dominant meteorological features result in the high pollution episodes. Hence, careful selection of representative episodes is essential to understand the dynamics of a particular region. Traditional statistical methods such as multivariate regression find limited applicability in air quality episode selection studies due to the presence of multiple prediction variables, lack of normalized distribution of data, and the existence of complex correlations between data.

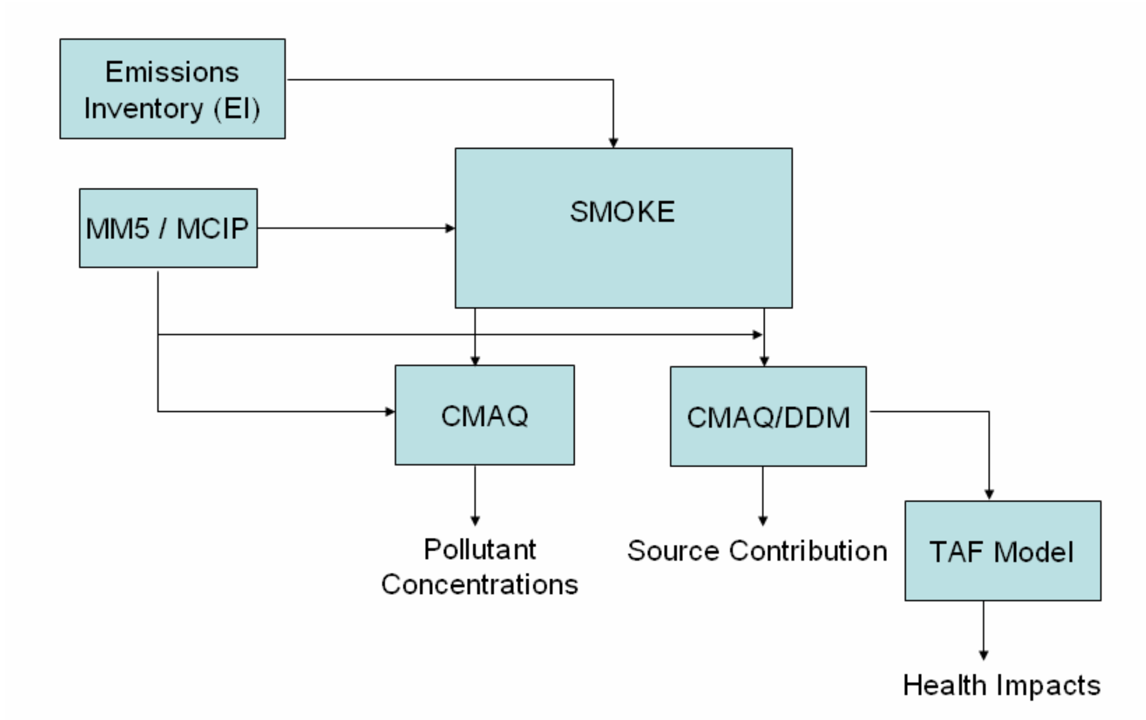

Figure 2.1 Modeling Approach

A different statistical procedure known as CART (Classification and Regression Trees) Analysis [2] is used in the analysis of categorical information (classification) or continuous information (regression). One of the characteristics of CART is that it represents the results in form of a decision tree. The structure of the tree is such that it can handle large amounts of data and makes interpretation easy. In essence, CART is a recursive binary partition technique. It divides a set of observations in subgroups taking as reference the value of a particular variable defined by the user (e.g., maximum daily ozone concentration). Each partition in the decision tree is conducted to minimize the classification error of the decision variable. In air quality studies, CART has been used to classify days with similar levels of pollution using a series of prediction variables as the classification criteria, e.g., wind direction and velocity, ambient temperature, relative humidity. CART is particularly useful in air quality episode selection due to its capacity to capture non-linearity in the existing relations of the data in complex databases. This technique has demonstrated its capacity to help in the selection of days with similar meteorological conditions that give rise to similar pollution levels using a formal procedure and eliminating the effects of meteorological variability. The CART software from Salford Systems was run to obtain decision trees to classify daily maximum ozone, CO and PM_{10} concentrations separately. Observations, both species concentrations, as well as meteorological parameters were taken from three air quality monitoring stations located close to the border region in Calexico (Ethel Street station, Grant Street station) and El Centro (9th Street station). The meteorological variables used are: maximum daily temperature, mean wind direction, mean wind velocity, mean solar radiation, maximum and minimum relative humidity. The years 2001 and 2002 were selected since the modeling team had already preprocessed data that could be used directly in the air quality system once the episodes had been selected, reducing the amount of resources that had to be dedicated of preprocessing large amounts of data. The results obtained from CART application were compared against time series plots to corroborate that the episodes selected in fact represented a continuum of days with relatively high pollutant concentrations levels [3].

Through the classification process it was found that the most important classification variable for 2001 ozone data were solar radiation (*SOLRAD*), followed by minimum relative humidity (*HUMIDMIN*), maximum temperature (*TMAX*), minimum temperature (*TMIN*), maximum humidity (*HUMIDMAX*), wind direction (*WNDDD$*), and wind intensity (*WNDSS*). For 2002 ozone data, the important classification variables were maximum temperature, followed by solar radiation, maximum humidity, and wind direction and velocity. August 23-26 represented Consecutive days with high O_3 concentrations with maximum of 0.142 ppmv, average 0.087 ppmv, and minimum 0.49

ppmv. Similarly, July 21-24 represented high levels of O_3 with an average concentration of 0.067 ppmv and a standard deviation of 0.011 ppmv.

Based on the CART analysis results, the summer episodes to be modeled were August 18-27, 2001, and July 17-24, 2001. These two episodes reflect high ozone events hence a third episode to represent high CO and PM levels during winter months was proposed. January 8, 14, 17, and 26 grouped together showed an average PM_{10} concentration of 55 $\mu g\ m^{-3}$, maximum of 214 $\mu g\ m^{-3}$ and a minimum of 18 $\mu g\ m^{-3}$. Therefore, a modeling episode of January 6-15, 2002 was selected.

2.3 Mesoscale Meteorological Scale 5 Model (MM5)

The Fifth generation Mesoscale Meteorological Model (MM5) is a meteorological model designed to simulate or predict the mesoscale atmospheric circulation[4]. The model consists of several auxillary programs such as TERRAIN, REGRID, LITTLE_R, INTERP_F, MM5 that are co-related to give the required meteorological output for use in air quality models. The following discussion gives in brief the functionalities of the various programs that form the meteorological model.

TERRAIN: This program horizontally interpolates the regular latitude-longitude, elevation, and vegetation/landuse data onto the model. Depending on the land surface model (LSM), additional fields such as vegetation fraction, soil temperature etc will be generated. According to the model domain defined, and the map projection specified, it generates terrain, landuse/vegetation and map-scale factors for all the model grids. For our current simulation, the USGS 25 Category land use coverage is utilized.

REGRID: Reads archived gridded meteorological analyses and forecasts on pressure levels, and interpolates those analyzes from its native grid and map projection to the horizontal grid and map projection as defined in the TERRAIN.

LITTLE_R: Develops the gridded pressure level meteorological data as a guess by objective analysis with reference from the observation data. The regridder output is the first guess used as the reference point. The output mainly consists of the 3-D pressure level analyses of winds, temperature, relative humidity, sea level pressure. The FDDA option is used for the nudging, as PXLSM model is used as the land surface model and which takes into account the three parallel pathways of evaporation from wet canopy, direct evaporation from the ground, and evapotranspiration to represent the humidity fluxes.

INTERPF: It handles the data transformation from the analysis programs such as RAWINS, LITTLE_R, and REGRID to the mesoscale model. It performs the vertical interpolation from the pressure levels to the sigma levels.

MM5: MM5 performs the time integration and numerical weather prediction, which forms the main input to the AQM's. MM5 has been used for a broad spectrum of theoretical and real-time studies, including applications to both predictive simulation and FDDA to monsoons, hurricanes, and cyclones. The main physics options in MM5 include that of cumulus parameterization, PBL/vertical diffusion, explicit moisture/microphysics, radiation, and surface schemes. The main physics options utilized for the current simulations is tabulated in Table 2.1.

Table 2.1. MM5 Parameterization Options

Parameter	**Description**	**Selected option**
IMPHYS	Explicit Moisture Scheme	Mix Phase
MPHYSTBL	Intrinsic Exponent for Calculating IMPHYS	Use lookup table for moist physics
ICUPA	Cumulus Schemes	Grell
IBLTYP	Planetary Boundary Layer	Pleim-Xiu
FRAD	Radiation Cooling of Atmosphere	Rapid Radiative Transfer Model (rrtm)
ISOIL	Multilayer Soil Temperature Model	Pleim-Xiu Land Surface Model
ISHALLO	Shallow Convection Option	No Shallow Convection

MCIP: The Meteorology-Chemistry Interface Processor (MCIP) links the MM5 data to the other parts of the MODELS-3 framework i.e. to SMOKE and the Chemical Transport Model (CTM) of CMAQ. The outputs produced by meteorological models are usually not in a format directly to be utilized by the air quality models, an interface processor is of utmost importance. MCIP performs operations such data format translation, conversion of units of various parameters, diagnostic estimations of parameters not provided, extraction of data for appropriate window domains, and reconstruction of meteorological data on different grid and layer structures. The interface processor provides a complete set of meteorological parameters to allow mass-consistent air quality computations for CTM in CMAQ and for emission computations in SMOKE. The output files generated consists of both two dimensional and three dimensional data. Also outputs consist of both time dependent and time-independent data.

2.4 SMOKE

The Sparse Matrix Operator Kernel for Emissions (SMOKE) [5] is used to prepare gridded emission files needed for air quality models with the help of emission surrogates from MIMS. Raw emission inventories are typically available as annual-total emissions values (area and point) and as average-monthly emissions values for mobile inventory (except California data, which is in annual format). However, AQM's typically require emissions data on an hourly basis, for each model grid cell, and for each modeled species. Consequently, emissions processing involves transforming the raw emission inventory through a) temporal allocation, b) chemical speciation, and c) spatial allocation, to achieve the input requirements of an AQM. SMOKE supports emissions processing for area, mobile, and point source and also includes biogenic emissions modeling through the Biogenic Emission Inventory System version 2 (BEIS2), which calculates the emission fluxes according to the landuse category and meteorological factors such as solar radiation. SMOKE also has the capability to process both criteria and toxic emissions data inventories.

Three sets of emissions inventories were utilized to perform the base case simulations. Simulations were performed for July 2001, August 2001, and January 2002 episodes using NEI 2001 combined with the 1999 BRAVO Mexican inventories, and the Six Border States Mexican inventory in January 2006[6]. The border states inventory have emission inventories from point, mobile, non-road, and non-point sources for the states of Baja California, Sonora, Chihuahua, Coahuila, Nuevo León, and Tamaulipas. Apart from the emission inventory files, the SMOKE program requires some additional files for processing of the inventories. Additional files such as emission surrogate ratios for Mexico were created using MIMS, and then merged with the US ratios for processing of the combined inventory [7]. Mobile source emissions for United States were processed using MOBILE6.

Some salient features during the processing of SMOKE:

- Though the surrogate ratios for the United States is complete with the USEPA recommended 89 categories for spatial surrogate generation; the shapefiles and subsequently the surrogate ratios were very limited for the Mexican region. The surrogate ratios provided along with the NEI 2001 for 36 km domain contained the Mexican surrogates that were created only on the basis of population. Hence, as an enhancement we created surrogates by spatial allocation based on population, highways, railroads, and marine ports for Mexico. The new spatial surrogates were created for the 12 km and 4 km domains, and were created using the Multimedia Integrated Management System (MIMS β). The shapefiles for creating the surrogates was obtained from USDOT: JWC U.S./Mexico Border Transportation Planning[8]. New surrogate codes of 990, 991, 992, 993, and 994 were assigned for Mexican population, highway, total railroads, airport points, and marine ports respectively. Consequently, the information was updated in the area and mobile cross reference file (amgref) for appropriate SCC's. An updated documentation file has been created to incorporate the new surrogate codes for the Mexican region.
- Even though EI data was available for the regions 202005 (Playas de Rosarito), 226071 (Benito Jurarez) and 226072 (San Ignacio Rio Muerto), population data for

these regions were unavailable. Since 226071 and 226072 were outside the study domains (12 km and 4 km), and the emission quantities being very small in these regions emissions processing was neglected from these regions. Emissions from 202005 were also emitted due to lower emissions.

- The mobile source emissions from Mexico were treated as Area emissions in SMOKE due to lack of VMT data for Mobile 6 at the time of processing the data.

Three sets of SMOKE simulations were further performed to obtain (1) point source emissions from Intergen, and Sempra units with Department of Energy (DOE) projected emissions, (2) Area source emissions if 100% of the roads in Mexicali were paved, (3) If 2.16 miles of Mexicali roads were paved to offset PM emissions from Intergen and Sempra units. Detailed description of the emissions is presented in Chapters 3 and 4.

2.5 CMAQ

The Community Multi-scale Air Quality (CMAQ) [1] model has the state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric O_3, fine particles, toxics, acid deposition, and visibility reduction, has been used to simulate the episodes. The CMAQ modeling system simulates various chemical and physical processes that are thought to be important for understanding atmospheric trace gas transformations and distributions. The CMAQ consists of the following interface processors: Initial conditions processor (ICON), Boundary conditions processor (BCON) , Photolysis rate processor (JPROC), Chemical-transport model processor (CCTM).

ICON: Initial conditions processor provides the concentration data for the pollutants, for the first hour of the simulation run. The data is created for all the grids. The input to the processor can be (a) time invariant set of vertical concentration, (b) three dimensional concentration files, (c) tracer species concentration.

The input data need not be present for all the species. If the initial values are not present; a default value of zero is taken. If the input utilized is the time independent data, the profiles developed for the RADM2 chemical mechanism according to the terrain following sigma pressure co-ordinates is utilized. The data are for the clean air conditions.

BCON: The boundary conditions processor creates the concentration data for the domain end grids only. The input methods specified for ICON are also valid for BCON. If the time invariant data is utilized, the input species concentration is a function of height, and is partially spatially independent for BCON. The profiles utilized in the time independent data are for the RADM2 chemical mechanism. BCON generates the output for 24 hrs or for the simulation period specified. For both ICON and BCON, the concentration values obtained are by linear interpolation for the vertical co-ordinate layer values.

JPROC: Calculates the photo-dissociation reaction rates for CMAQ. JPROC produces a clear sky photolysis rate look-up table that consists of photolysis rates at various altitudes, latitudes and hour angles. It is simulated for each day and depends on the chemical mechanism chosen. The method for setting photolysis rates follows that of RADM [9], with modifications by Stockwell, Middleton, and Chang [10]. The PHOT module of CMAQ produces the photolysis rates for individual grid cells by interpolating with the look-up tables. The PHOT module also uses parameterization to correct for the cloud cover photolysis rates.

CCTM: CCTM simulates the relevant and major atmospheric chemistry, transport and deposition processes involved throughout the modeling domains. It takes into account the factors of advection/diffusion, gas phase chemistry, plume-in grid modeling, particulate modeling and visibility, cloud processes and photolysis rates.

2.6 CMAQ-Decoupled Direct Method (DDM)

Sensitivity analysis is vital for secondary pollutants such as ozone, whose sensitivity to emissions of its precursors primarily nitrogen oxides (NO*x*) and volatile organic compounds (VOCs) changes in magnitude and sign depending upon spatio-temporally varying factors [11]. To understand the impacts of emissions from various sources on species concentrations, the first order semi-normalized sensitivities were obtained using CMAQ along with Direct Decoupled Method (DDM)[12-15]. Sensitivity of C_i to emission perturbations can be found as follows:

$$S_{i,j}^{(1)} = \frac{\partial C_i(x,t)}{\partial \mathrm{E}_i}$$

where E_j is the relative emission perturbation. CMAQv4.3/DDM and CMAQ v 4.5 with DDM 3D/PM [15] was used to simulate gaseous, as well as aerosol species sensitivities for the 12 km domain during August 2001 and January 2002 episodes. Further description of the implementation of DDM is presented in Chapters 3 and 4.

2.7 TAF Model

The Tracking and Analysis Framework (TAF) model [16] is being used to study the health impacts from emissions of the two power plants, Intergen and Sempra over the border region. The objective of TAF is to bridge the gap between science and policy. The primary objective in the development of TAF was to help National Acid Precipitation Assessment Program (NAPAP) fulfill its mandate under the 1990 Clean Air Act Amendments. It was developed to (a) evaluate the status of implementation, the effectiveness, and the costs and benefits of the acid-deposition control program created by Title IV of the Act, and (b) to determine whether additional reductions in deposition are necessary to prevent adverse ecological effects. This bridge between science and policy is designed to facilitate discussion in both directions: Policy should be informed by the best available science; and scientific research should be focused on those issues most relevant to the policy questions of primary concern. Accordingly, TAF has a set of secondary objectives: to support coordination among scientists, to help them share, review, and assess models and data, to support communication with policy makers, about key results and insights, to ensure that the model reflects their concerns, and to provide guidance for prioritizing research needs based on policy concerns and the most critical sources of uncertainty and gaps in data. Although originally developed to examine the effects of acid rain precursors, it is now used to examine all types of air pollution effects.

Health effects and monetary valuation are estimated in TAF using pollutant concentration data and demographics data. TAF 2006 uses O_3 and $PM_{2.5}$ for studying health effects of pollution. TAF is not a single model, but rather a flexible framework for modeling an integrated assessment. As new policy questions emerge, information needs will evolve. To meet these challenges, the TAF framework is designed to accept replacements so that other modules can be slotted in to replace for existing modules or to expand the model to address new issues. A snapshot of the TAF model is presented in Figure A.1

The work on the health impacts is being solely conducted at RFF by Dr. Allen Blackman and Zhuxuan You. As the work on the estimation of health impacts using the TAF model is in progress, we will limit our discussion only to one of the inputs to the TAF model i.e., O_3 and $PM_{2.5}$ concentrations, in this thesis.

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CHAPTER 3

AIR TRANSPORT AND POLLUTANT INTERACTIONS BETWEEN LOS ANGELES, MEXICALI-CALEXICO, AND TIJUANA-SAN DIEGO

3.1 Introduction

Trans-boundary air pollution across United States and Mexico is a rising issue due to increased commercial and industrial activities in the border regions. Current air quality trends in Mexico indicate that urban centers like Mexico City, Monterrey, Guadalajara, Toluca, Ciudad Juarez, Mexicali and Tijuana continue to exceed the Mexican Air Quality Standards for ozone (O_3) and particulate matter less than 10 µm in diameter (PM_{10}), while other cities are starting to show warning signs of future air quality problems [1]. The western border between Mexico and the United States has two major urban industrial regions, Tijuana-San Diego and Mexicali-Calexico (Imperial Valley) (Figure 3.1). Tijuana-San Diego has been a border economic area for quite sometime, while over the last fifteen years Mexicali has been one of the fastest-growing cities in Mexico in terms of industrial development, job creation, and energy demand. The resulting increase in air pollution and environmental degradation presents challenges as well as opportunities for achieving sustainable and socially responsible economic growth. Imperial Valley has also been designated by USEPA as O_3 non-attainment for many years now.

Harmful contaminants in the border region originate from a number of sources, including motor vehicles, unpaved roads, farms, power plants, and factories. Geothermal power plants, light manufacturing operations, waste disposal sites, mining, and aggregate handling are also located near the borders. The resulting air pollution has been linked to high rates of asthma and respiratory diseases on both sides of the border [2].

Mexicali and the Imperial Valley have similar environmental regulations for carbon monoxide (CO), O_3, and PM_{10}, and both regions are out of compliance for these pollutants.

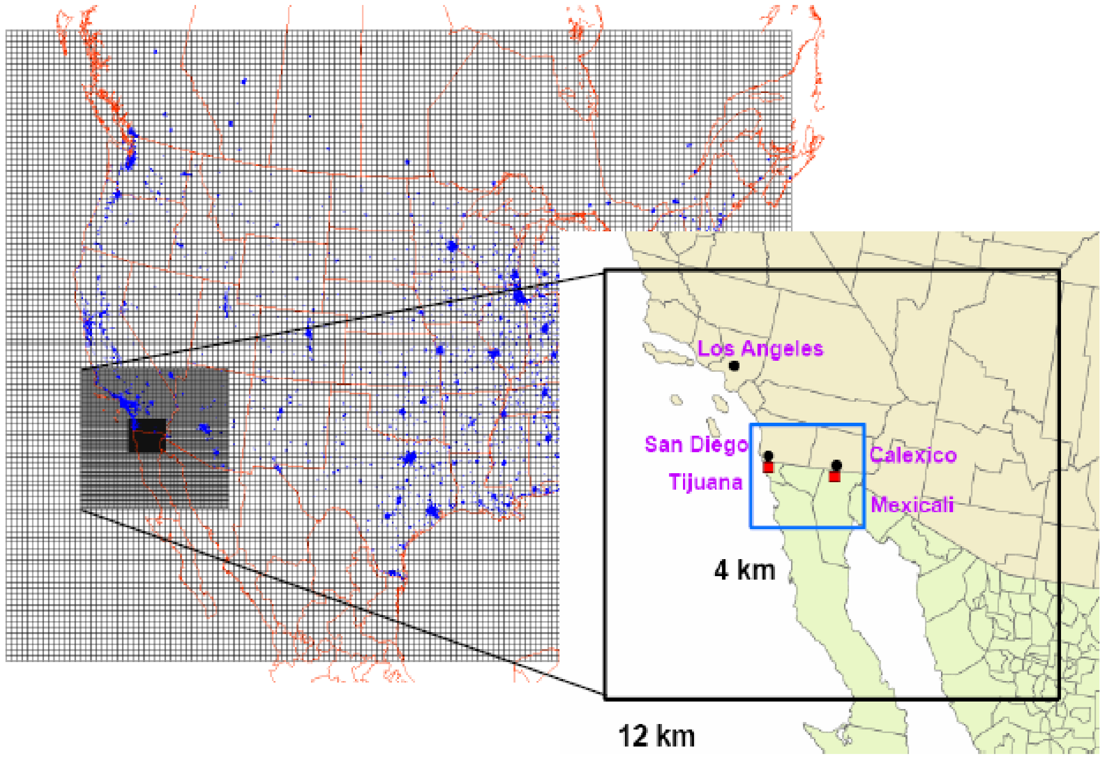


Figure 3.1 Modeling domain representing 36 km, 12 km, and 4 km resolutions. Inset shows primary areas studied inside the 12 km and 4 km domains

Several studies have been conducted in the past 15 years in order to understand the pollutant composition, spatial variability, and sources in the Mexicali-Calexico region [3-5]. These studies are limited to understanding the PM_{10} dynamics and the need to study the dynamics of O_3 and particulate matter less than 2.5 μm ($PM_{2.5}$) over the region still remains. In this chapter, we describe pollutant formation and pollutant interactions between the three regions of Mexicali-Imperial Valley, Tijuana-San Diego, and Los Angeles using the Community Multiscale Air Quality (CMAQ) model [6] for analyzing the formation of secondary species, and transport of both primary and secondary pollutants during three pollution episodes of July 15-23, 2001, August 18-27, 2001, and January 6-

15, 2002. Impacts of particular sources/source contribution from within the region and from other regions during summer (August 2001) and winter (January 2002) episodes is conducted using the sensitivity analysis approach with CMAQv4.3/DDM [7-9].

3.2 Approach

Models-3 framework i.e., three models required for air quality modeling, which are (1) meteorological model to simulate the dynamics in the atmosphere, (2) emissions model to simulate the primary emissions within the region of interest, and (3) the chemical mechanism model to simulate the complex chemical reactions/interactions occurring between varying pollutants, is utilized. The employed meteorological model is the Fifth generation Mesoscale Meteorological (MM5) model, the emission processor utilized is the Sparse Matrix Operator Kernel Emissions (SMOKE), and CMAQ is used to simulate secondary pollutant formation and chemical transport.

3.2.1 CMAQ Model

CMAQ is an Eulerian photochemical model that simulates the emissions, transport, and chemical transformations of gases and particles in the troposphere [6]. Similar to other photochemical models, CMAQ solves the species conservation equation given as follows:

$$\frac{\partial C_i}{\partial t} = -\nabla \cdot (\mathbf{u} C_i) + \nabla \cdot (\mathbf{K} \nabla C_i) + R_i + E_i \qquad (3.1)$$

Where, C_i is the concentration of species i, u is the fluid velocity, K is the eddy diffusivity tensor, R_i is the net rate of generation of specie i, E_i is the emission rate of species i. Meteorological parameters such as **u** and **K** in Equation 3.1, as well as additional information used to define reaction rates are developed from a corresponding meteorological model MM5 [10]. The vertical structure has thirteen layers with its top at about 15.9 km above ground. Seven layers are below 1 km and the first layer thickness is set at about 18 meters. The Meteorology Chemistry Interface Processor (MCIP v2.3) is used to convert MM5 output data into model ready format. 36 km modeling grid domain is considered as the mother domain, and further nest-down operation yields the boundary conditions required for 12 km domain simulations discussed in this paper (Figure 3.1). The 12 km resolution grid having 84 columns and 75 rows is nested over regions of Southern California, and northern part of Baja California encompassing Mexicali and Tijuana.

The representation of maps is in Lambert Conformal Conics projection with center co-ordinates at (40,-97) in degrees. The first three days during each episode are considered as model spin-up days or model stabilization period.

3.2.2 Emissions Modeling

The Sparse Matrix Operator Kernel for Emissions (SMOKEv2.1) [11] is used to prepare gridded emission files needed for air quality models. Three sets of emissions inventories were utilized to perform the base case simulations. Simulations were performed for July 2001, August 2001, and January 2002 episodes using National Emissions Inventory (NEI) 2001 combined with the 1999 BRAVO Mexican inventories, and the Six Border States Mexican inventory in January 2006[12]. The border states inventory have emission inventories from point, mobile, non-road, and non-point sources for the states of Baja California, Sonora, Chihuahua, Coahuila, Nuevo León, and Tamaulipas. Apart from the emission inventory files, the SMOKE program requires additional files for processing of the inventories. Additional files such as emission surrogate ratios for Mexico were created and then merged with the US ratios for processing of the combined inventory [13]. Mobile source emissions for United States were processed using MOBILE 6. The mobile source emissions from Mexico have been treated as area emissions in SMOKE due to lack of Vehicle Miles Traveled (VMT) data for MOBILE 6 processing at the time of simulations. SAPRC99 was used as the chemical mechanism within the model [14]. The emission distribution of area, mobile, point, and biogenic sources for the three regions from the above mentioned inventory data is represented in Figure 3.2. The primary contribution of PM in the Mexicali-Calexico is from area sources that are dominated by wood-fuel combustion, agricultural burning, and paved and unpaved road dust.

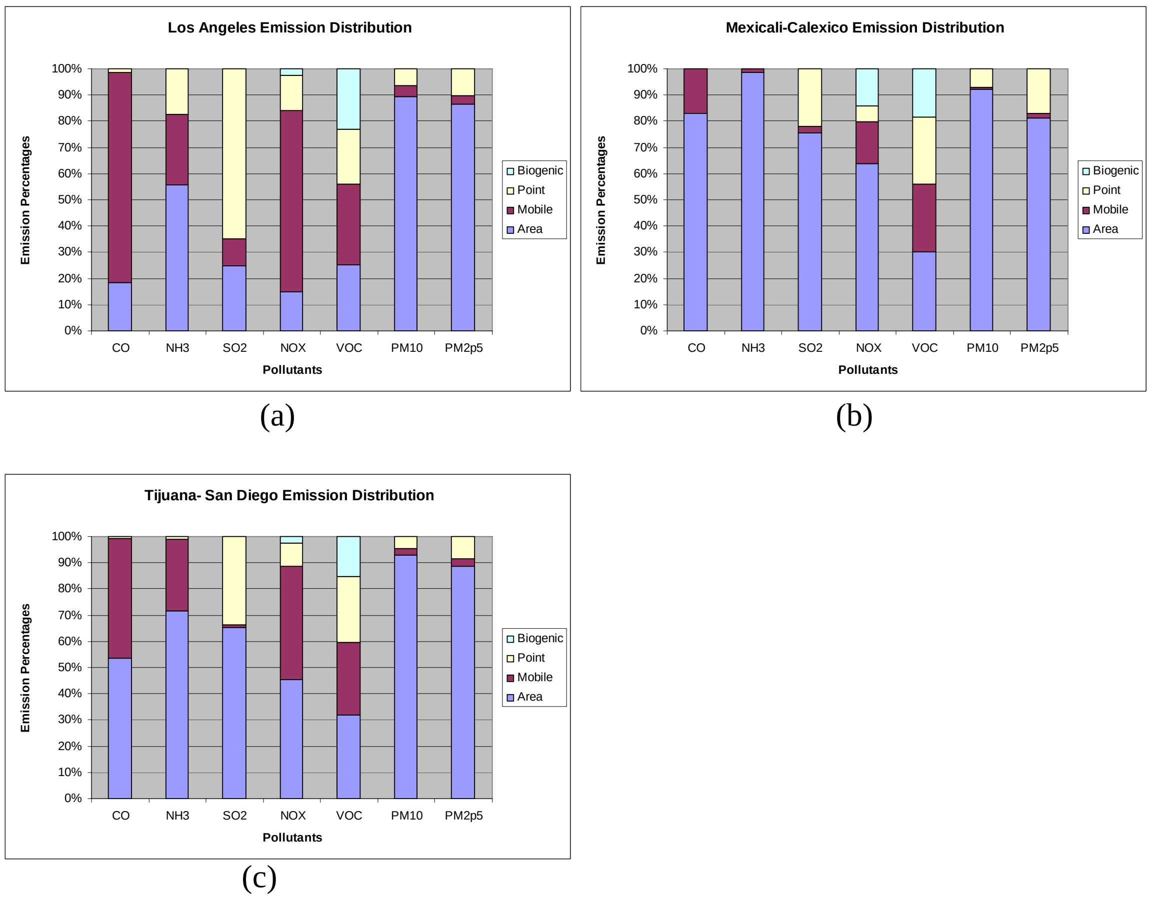


Figure 3.2 Emission distributions in (a) Los Angeles, (b) Mexicali-Calexico, (c) Tijuana-San Diego

Area sources contribute to 83% of CO, 98% of Ammonia (NH_3), 75% of $SO_{2,}$ 64% of NOx, 30% of VOC's, 92% of PM_{10}, and 81% of $PM_{2.5}$ in the Mexicali-Calexico region. As expected in Los Angeles, the primary emitters are mobile sources. Tijuana-San Diego show high contributions from both area, as well as, mobile sources.

3.2.3 CMAQ Decoupled Direct Method (CMAQ DDM)

To understand the impacts of emissions from various sources on species concentrations, the first order semi-normalized sensitivities were obtained using CMAQv4.3/DDM [7, 9]. Sensitivity of C_i to emission perturbations can be stated as follows:

$$S_{i,j}^{(1)} = \frac{\partial C_i(x,t)}{\partial \mathrm{E}_i} \qquad (3.2)$$

where E_j is the relative emission perturbation. Areas of interest are divided into three different zones: Mexicali-Calexico (abbreviated as MC), Tijuana-Tecate-San Diego (abbreviated as TS), and Los Angeles-Riverside-Orange-Ventura (abbreviated as LA). CMAQ v4.3/DDM is used to calculate sensitivities (i.e., gaseous pollutant concentrations to emissions of NOx and VOC) from 1) LA mobile sources, 2) LA area sources, 3) LA point sources, 4) MC area sources, 5) Mexicali mobile sources, 6) Calexico mobile sources 6) TS area sources, 7) Tijuana mobile sources and 8) San Diego mobile sources. Discussion in later sections will be focused towards area and mobile sources as they are the primary pollutant emitters in MC and TS region. Additionally, in order to estimate impacts over the region from $PM_{2.5}$ emissions in Mexicali-Calexico and Tijuana-San Diego CMAQ4.5/DDM3D-PM was simulated. The simulations calculated PM sensitivities (i.e., pollutant concentrations to $PM_{2.5}$ emissions) from 9) MC area sources, 10) MC mobile sources 11) MC point sources, 12) TS area sources, 13) TS mobile sources, and 14) TS point sources.

3.3 Results and Discussion

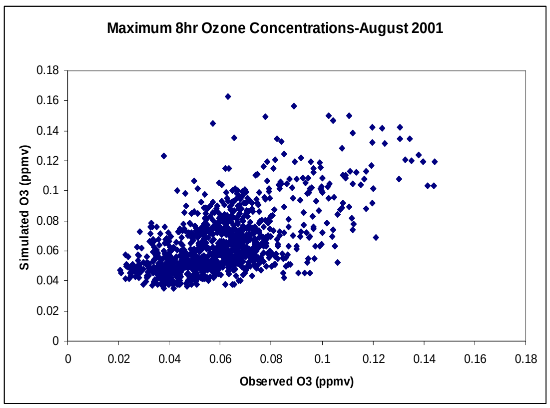
3.3.1 Performance Characteristics

Domain-wide episode performance characteristics are determined to ascertain the confidence of the simulation results. Table 3.1 represents the average performance characteristics of the 12 km domain in terms of Mean Bias Error (MBE), Root Mean Squared Error (RMSE), Mean Normalized Bias (MNB), and Mean Normalized Error (MNE). R-squared (Square of the correlation co-efficient) value of 0.37 is obtained between observed and simulated maximum 8 hr O_3 concentrations in the 12 km domain during the summer episode of August 2001 (Figure 3.3a). During the winter episode of January 2002, R-squared value of 0.347 is obtained between observed and simulated daily average $PM_{2.5}$ concentrations in the 12 km domain (Figure 3.3b). Representative sites in each of the three regions were chosen in order to compare between predicted and observed pollutant concentrations (Figure A.2).

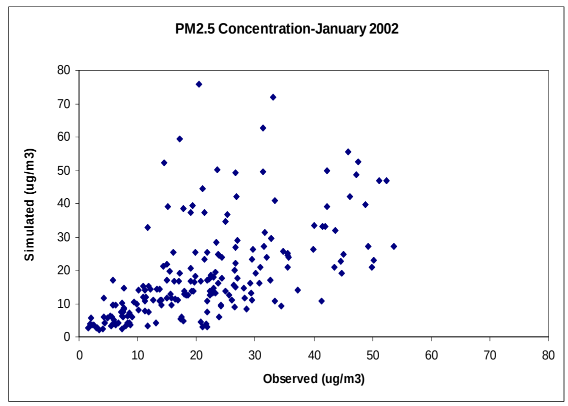
Table 3.1 Average performance characteristics of 12 km domain during August 2001, July 2001 and January 2002 episodes

		MBE	RMSE	MNB	MNE
August-01	**Ozone**	-1.64E-03	1.60E-02	-2.10E-01	1.97E+01
	CO	-3.52E-01	6.56E-01	-1.86E+01	6.32E+01
	NOx	-1.25E-02	2.52E-02	-3.49E+01	7.42E+01
	SO2	-1.40E-03	5.40E-03	-1.94E+01	8.77E+01
	PM2.5	-6.76E+00	9.14E+00	-3.69E+01	3.92E+01
	PM10	-3.00E+01	3.57E+01	-7.62E+01	7.62E+01
July-01	**Ozone**	-9.19E-02	1.76E-01	-1.83E+01	6.12E+01
	CO	-1.43E+00	1.97E+00	-2.20E+01	5.68E+01
	NOx	-6.18E+00	7.58E+00	-3.10E+01	6.00E+01
	SO2	-5.31E+00	6.53E+00	-2.92E+01	6.02E+01
	PM2.5	-7.10E+00	8.72E+00	-3.33E+01	6.30E+01
	PM10	-8.12E+00	9.97E+00	-3.53E+01	5.95E+01
January-02	**Ozone**	2.86E-03	7.76E-03	6.96E+00	1.41E+01
	CO	-7.33E-01	1.33E+00	-2.65E+01	7.31E+01
	NOx	-3.99E-02	7.98E-02	-3.46E+01	7.60E+01
	SO2	-1.10E-03	5.40E-03	-2.96E+01	7.44E+01
	PM2.5	-2.54E+00	1.01E+01	-4.59E+00	3.72E+01
	PM10	-2.53E+01	3.21E+01	-5.61E+01	6.17E+01

Peak O_3 concentrations were observed on August 26th in the 12 km domain during August 2001 episode, and maximum values were observed in the Los Angeles area. In Los Angeles, peak concentrations of 189 and 190 ppbv were observed at Azusa and Glendora Laurel sites respectively [15]. These sites are located in the San Gabriel valley and come under the same 12 km grid cell. Simulated concentrations correlated well with the observed concentrations at Azusa (MBE 0.0050, MNB 12.19) and Glendora Laurel (MBE 0, MNB 3.49) on most days. However, in the model application, the simulated



(a)



(b)

Figure 3.3 (a) Scatter plot comparing maximum 8 hr O_3 Concentrations between observations and simulated results during the summer episode, r^2= 0.37, (b) Scatter plot comparing $PM_{2.5}$ concentrations between observations and simulated results during the winter Episode, r^2=0.347

peak O_3 concentration was 55 ppbv lower at Azusa and 56 ppbv at Glendora Laurel (Figure 3.4a,b). All the time steps expressed in this thesis are in UTC timings. Pacific Daylight time (PDT) is followed during July and August episodes (i.e., UTC minus 7 hrs), while Pacific Standard Time (PST) is followed during the January episode (i.e., UTC minus 8 hrs).

Peak concentrations in Calexico were observed at Ethel Street (MBE -0.0044, MNB -2.99), and East Calexico (MBE 0.0045, MNB 11.99) sites. Observed data was not available in Mexicali to compare with simulations. Calexico and Mexicali being adjacent to each other in the border region, we can assume that the pollutant concentrations will be similar in these regions. The inability to capture the minimums in Ethel Street and Calexico East sites can be attributed to the fact that both these locations are located very close the roadways, hence experience strong O_3 sinks in the night time due to its reaction with NO which the model is unable to capture using a 12 km grid (Figure 3.4c, d).

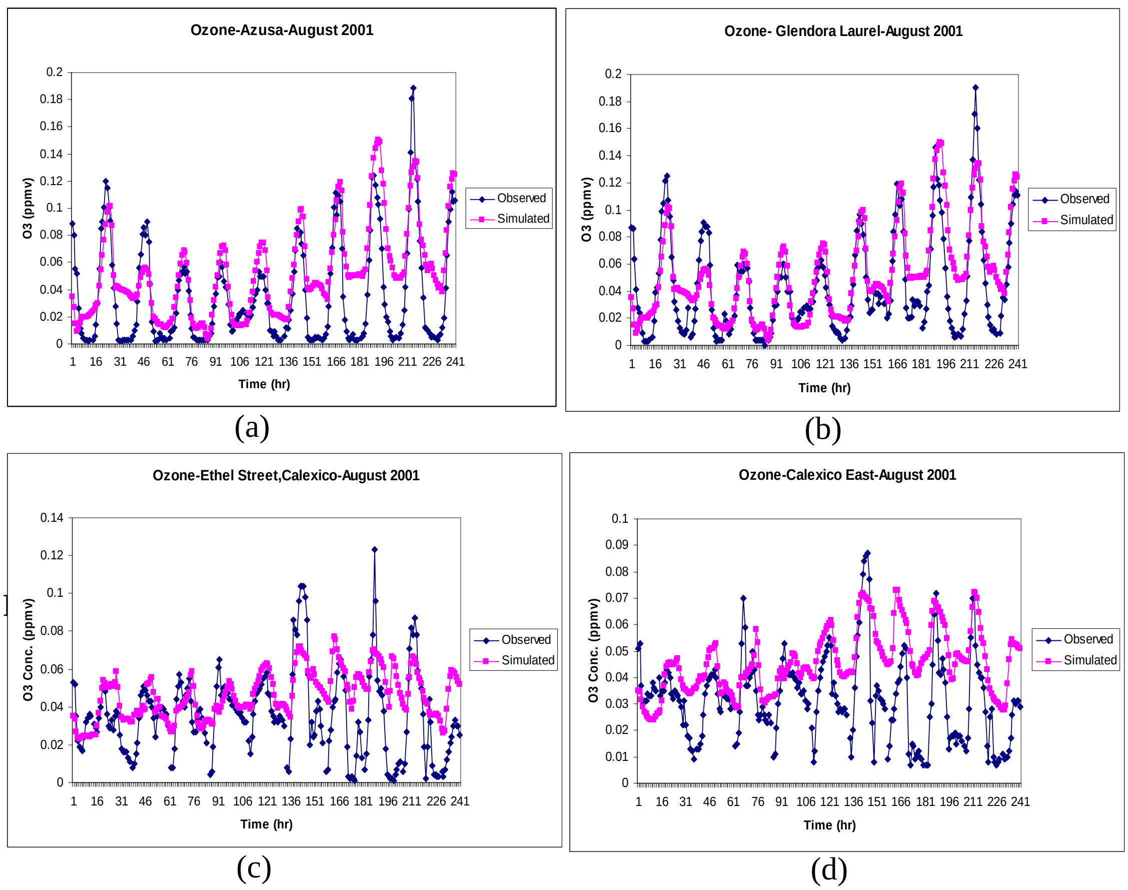


Figure 3.4 Observed vs. Simulated O_3 concentrations at representative sites in Los Angeles, and Mexicali Calexico during August 2001 at (a) Azusa, Los Angeles (b) Glendora Laurel, Los Angeles, (c) Ethel Street, Calexico, (d) Calexico East site, Calexico

3.3.2 July 2001 Episode

During the July 2001 episode, a peak of 125 ppbv O_3 is simulated in the Los Angeles area on July 23, 23:00 hrs UTC (Figure 3.5d). The plume from Los Angeles can be seen transported towards Nevada (Figure 3.5a, b, c). Plumes ranging up to 78 ppbv O_3 emerge from San Diego-Tijuana and travel eastwards and are seen to impact the

Mexicali-Calexico region (Figure 3.5a, b, c). Peak $PM_{2.5}$ concentrations of over 50 µg m^{-3} are simulated in Los Angeles area on July 15th, while the concentrations do not exceed 15 µg m^{-3} in Tijuana-San Diego and Mexicali-Calexico during the July episode.

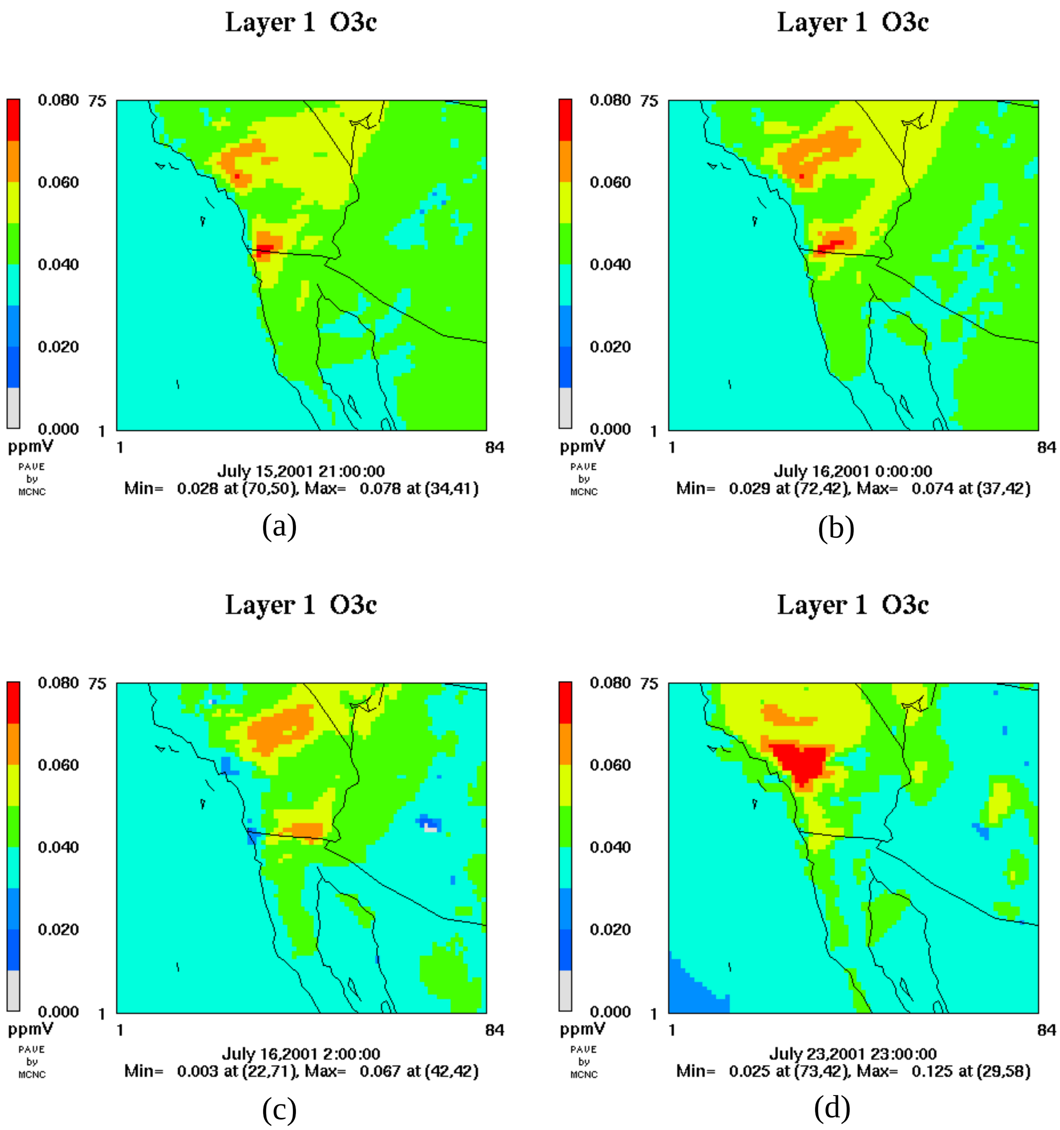


Figure 3.5 (a) (b) (c) Transport of O_3 plumes from Los Angeles and Tijuana-San Diego traveling eastwards Nevada and Mexicali-Calexico respectively, (d) Peak concentration of 125 ppbv O_3 simulated in Los Angeles on July 23, 2001

3.3.3 August 2001 Episode

3.3.3.1 Base Case

On August 24th (20:00 hrs UTC), strong O_3 plumes start to develop, and plumes from Mexicali-Calexico and Los Angeles almost converge (Figure 3.6a). At the same time plumes from Tijuana-San Diego build up as well and go eastwards towards Mexicali-Calexico (Figure 3.6b).

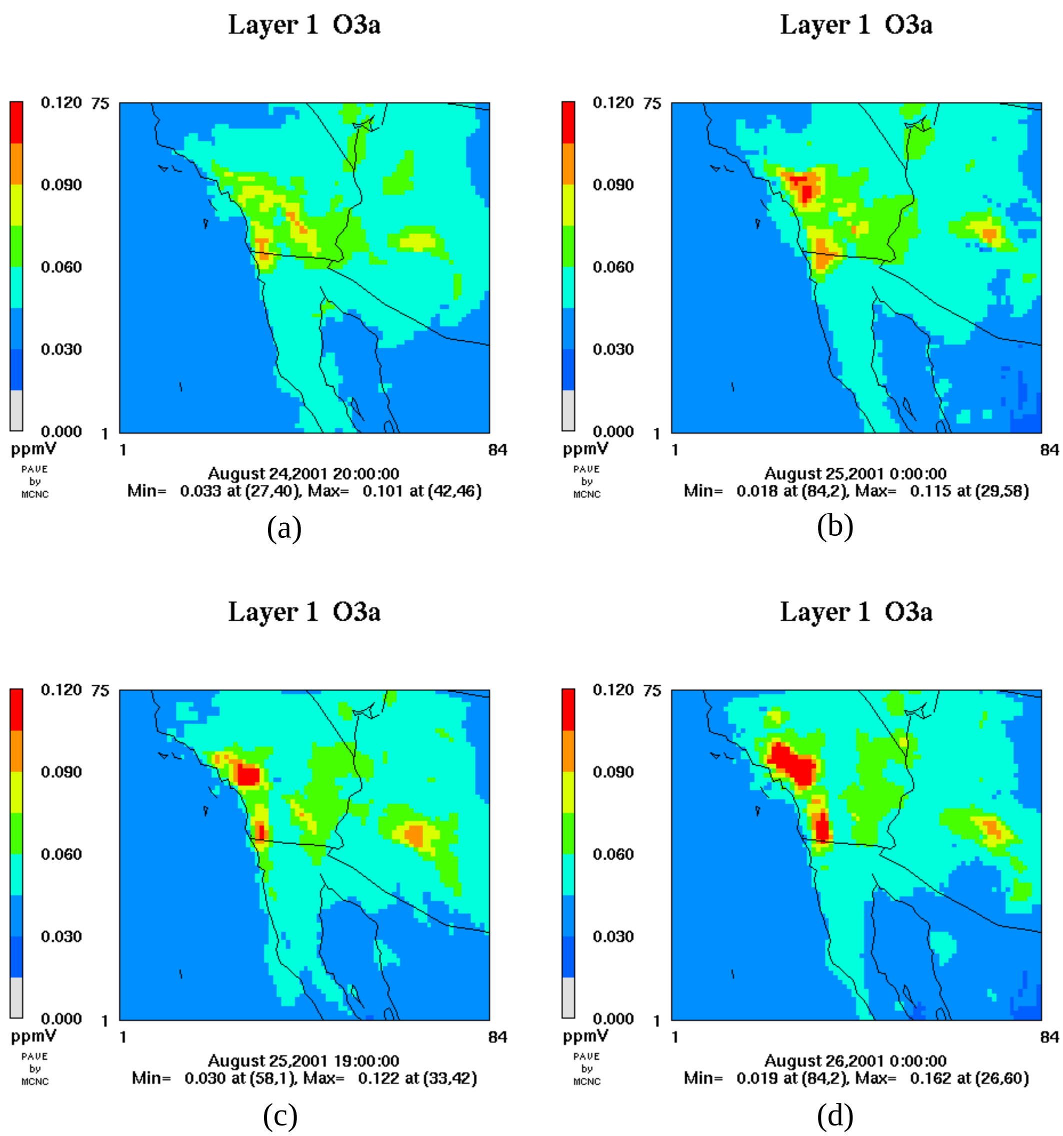


Figure 3.6 (a) Emerging O_3 plumes from Los Angeles and Mexicali-Calexico meeting, (b) O_3 plumes from Tijuana-San Diego moving eastwards along the border, (c) High O_3 levels seen in the three regions, (d) Peak O_3 Concentrations near Glendora Laurel on August 26th (00:00 hrs UTC)

Similar patterns start to emerge on August 25th (19:00 hrs UTC) (Figure 3.6c), and the peaks reach to 162 ppbv in the Los Angeles area on August 26th (00:00 hrs UTC) (Figure 3.6d). A peak concentration of 162 ppbv is reached at grid location (26, 60) which is located two grids (northwest) away from the grid having Glendora Laurel (simulated peak of 144 ppbv). However, there is no monitoring station present in that location, hence direct comparison with observed data is not possible. Similar to the July episode, O_3 plumes from San Diego-Tijuana border area are transported eastward towards Mexicali-Calexico during the August episode as well. Peak $PM_{2.5}$ concentration of 100 μg m^{-3} is seen close to Los Angeles area on August 25th (Figure 3.7). In Mexicali-Calexico region, Mexicali showed a peak of 42 μg m^{-3} on August 25th (14:00 hrs UTC).

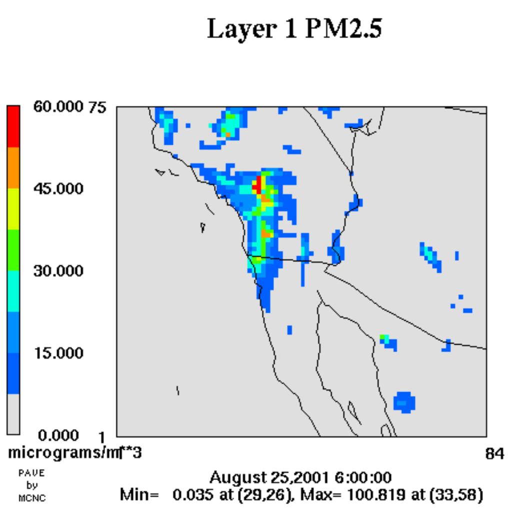


Figure 3.7 Peak $PM_{2.5}$ concentration of 100 μg m^{-3} near Los Angeles area during August 2001 Episode

<u>3.3.3.2 Source Contribution during August 2001 Episode</u>

In order to understand the source contribution during the August 2001 episode, sensitivities were simulated using CMAQ4.3 /DDM as described in section 3.2.3. LA mobile sources made a contribution of 44 ppbv on the surrounding region i.e., east of Los Angeles city towards Glendora Laurel and Azuza on August 26 (00:00 hrs UTC) (Figure 3.8c). Presence of high concentrations of NOx results in negative sensitivities up to – 46 ppbv in urban Los Angeles (Figure 3.8a). As seen in the base case simulations where

O_3 plumes from LA, Mexicali-Calexico and Tijuana formed a triangle over southern California, O_3 plumes are being transported towards Mexicali-Calexico with levels up to 10 ppbv above the surrounding region (Figure 3.8a). Due to the north easterly direction of the winds, plumes also reach Grand Canyon National Park area, again with levels of about 10 ppbv above the surroundings (Figure 3.8d). LA area sources contribute up to 8 ppbv of O_3 in Riverside area. Area sources in Los Angeles city emit considerable NOx, which lead to negative sensitivities of up to -36 ppbv of O_3 in Los Angeles itself (Figure 3.9).

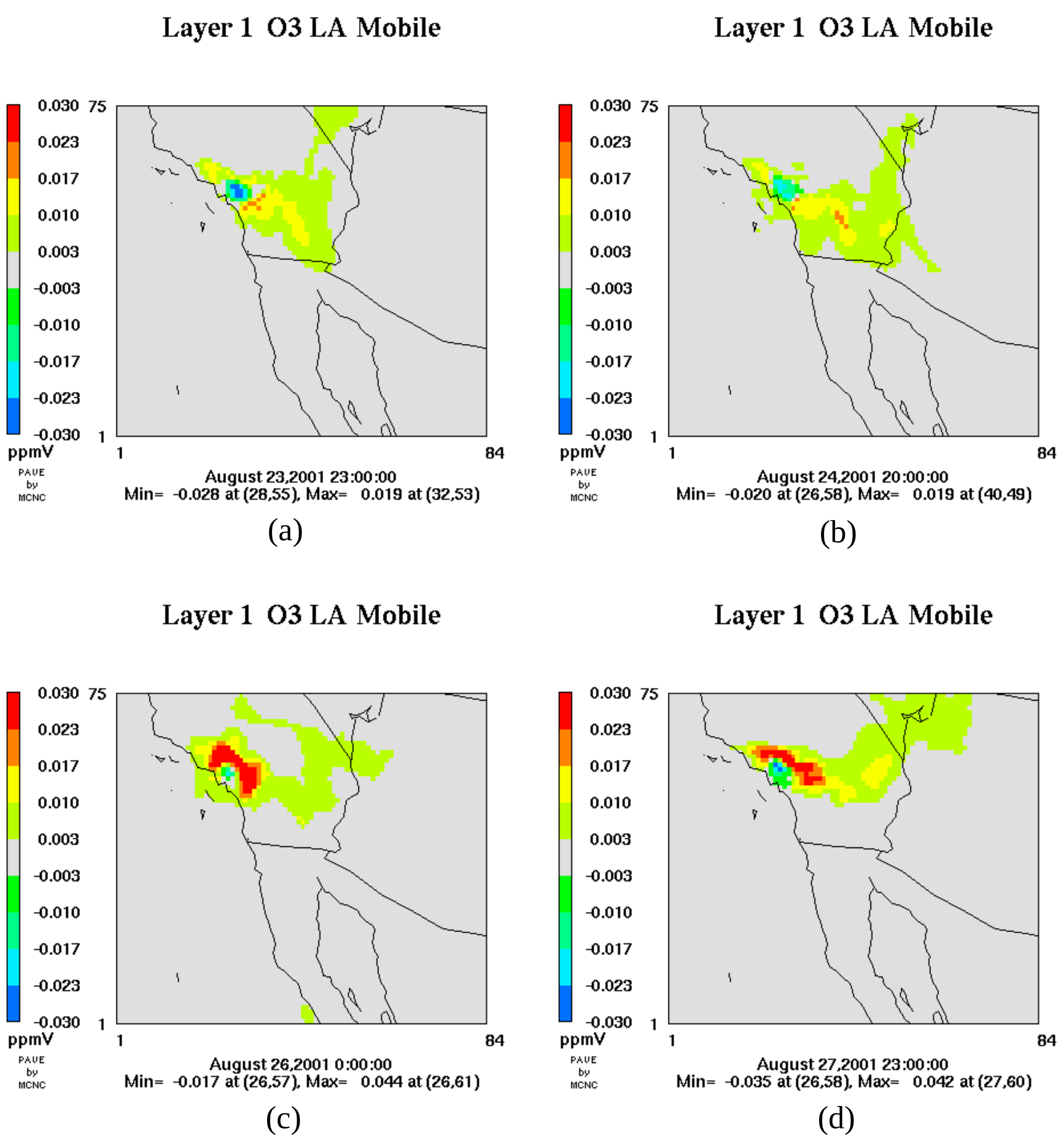


Figure 3.8 (a) (b) O_3 plumes emerging from LA mobile sources impacting Mexicali-Calexico and San Diego, (c) Peak O_3 contribution of 44 ppbv east of Los Angeles city, (d) Plumes being carried away towards Grand Canyon National Park, in Summer

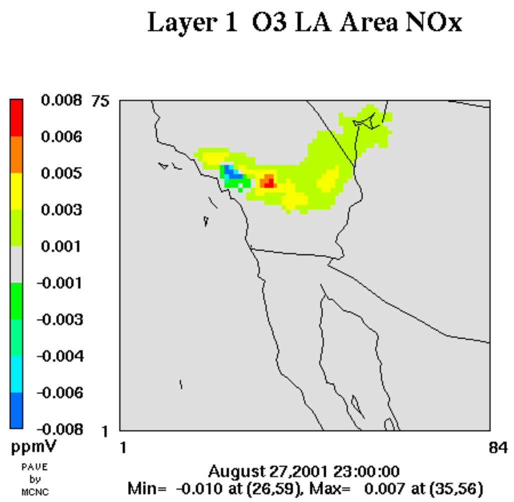


Figure 3.9 LA area sources impacting O_3 levels across the region during summer 2001

Mobile traffic passing through Mexicali's border crossings is of concern. However, the mobile contribution to O_3 is found to be small in the simulation results. The impact from Mexicali vehicles alone is very small, with a peak impact of only 1.3 ppbv over Calexico and Mexicali (Figure 3.10). Emission inventory underestimates can be a potential reason for low simulated impacts.

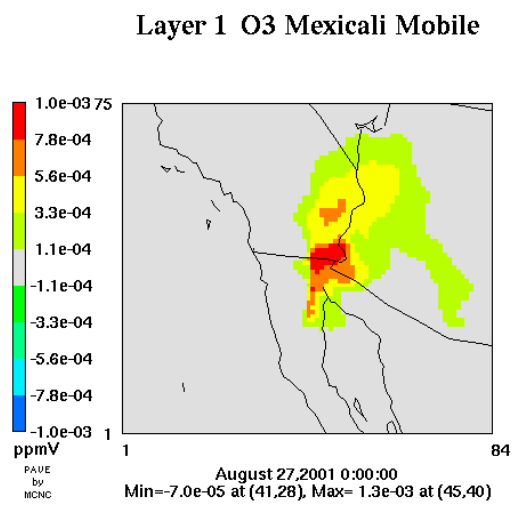


Figure 3.10 Contribution to O_3 concentrations from Mexicali mobile sources

The maximum impact from Calexico mobile sources is 2 ppbv of O_3 seen over the Calexico region itself, and the border between California and Arizona (Figure 3.11). The primary areas of mobile emissions are the two border crossing areas (seen in blue as negative sensitivities).

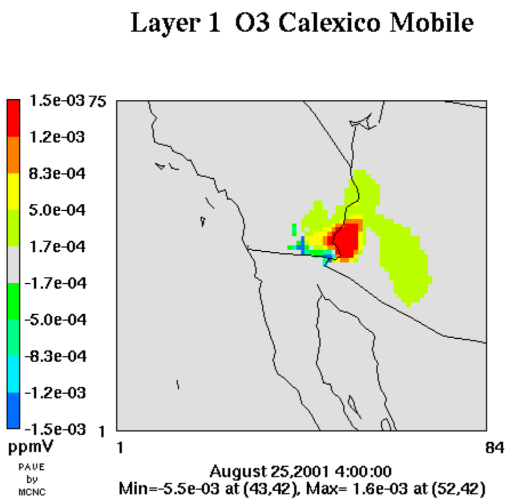
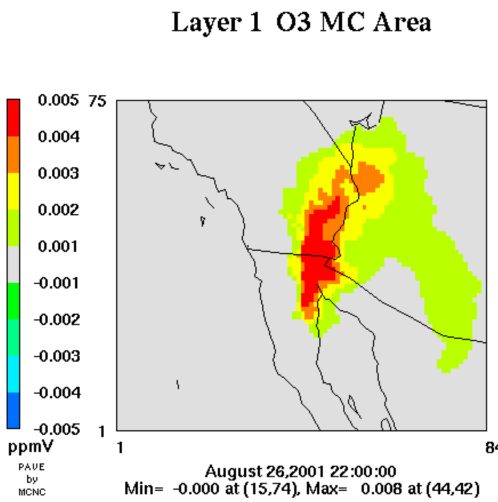


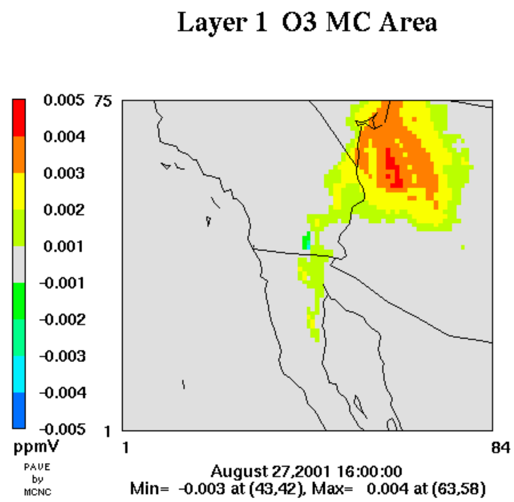
Figure 3.11 Mobile emissions from Calexico having maximum impact of 2 ppbv O_3 on the Calexico region during summer episode

Area sources in MC contribute a simulated maximum of 8 ppbv O_3 during the summer episode (Figure 3.12a). The plume can be seen encompassing California, and the border regions of California-Arizona. O_3 impacts up to 4 ppbv in the Grand Canyon area can be attributed to area sources in the Mexicali-Calexico region (Figure 3.12b).

Area sources from TS have a peak impact of 40 ppbv of O_3 over the San Diego area and this plume is carried eastwards in United States close to the border region. The plume emerging from Tijuana is transported in the southeast direction into inner Baja California and impacting up to 20 ppbv of O_3 (Figures 3.13a,b). Also, on August 26th, the plume emerging from Tijuana-San Diego region is transported eastwards towards Calexico, thus adding O_3 to the already polluted air in Calexico and Mexicali (Figure 3.13c,d).



(a)



(b)

Figure 3.12 (a) Secondary formation of O_3 emerging from MC area sources, (b) MC area sources contributing upto 4 ppbv of O_3 in the Grand Canyon area

Tijuana mobile source impacts reach up to 6 ppbv on both sides of the border depending on the wind direction (Figure 3.14b, c). Since the dominant wind pattern being more towards northeast, O_3 is transported through the California-Baja California border towards Calexico (Figure 3.14a, c). Tijuana mobile sources impacts up to 3 ppbv of O_3 in Mexicali-Calexico (Figure 3.14a).

Mobile sources from San Diego contribute up to 26 ppbv of O_3 in the region itself, and also over the park areas such as Anza Borrego Desert State Park located southeast of San Diego (Figure 3.15a). The base case scenario showed O_3 plumes from Tijuana-San Diego area transported to Calexico-Mexicali. A contribution of up to 11 ppbv of O_3 in Calexico-Mexicali can be attributed to the high density of vehicles in and around the San Diego region (Figure 3.15b). This contribution is higher than the contribution from Calexico-Mexicali mobile sources.

The peak $PM_{2.5}$ concentrations simulated over MC region was 42 μg m^{-3}. Of this, MC area sources contributed to 21 μg m^{-3} of primary $PM_{2.5}$. About 50% of the $PM_{2.5}$ emissions in MC can be attributed directly to area sources in MC during August 2001. $PM_{2.5}$ contribution from MC mobile sources was very small, with peak contributions less than 1 μg m^{-3}. MC point sources contributed the remaining share of up to 7 μg m^{-3}.

Simulations found similar results for Tijuana-San Diego with contributions ranging upto 33 µg m^{-3} of $PM_{2.5}$ from TS area sources, less than 2 µg m^{-3} from mobile sources, while the point sources in the region contributed up to 13 µg m^{-3}.

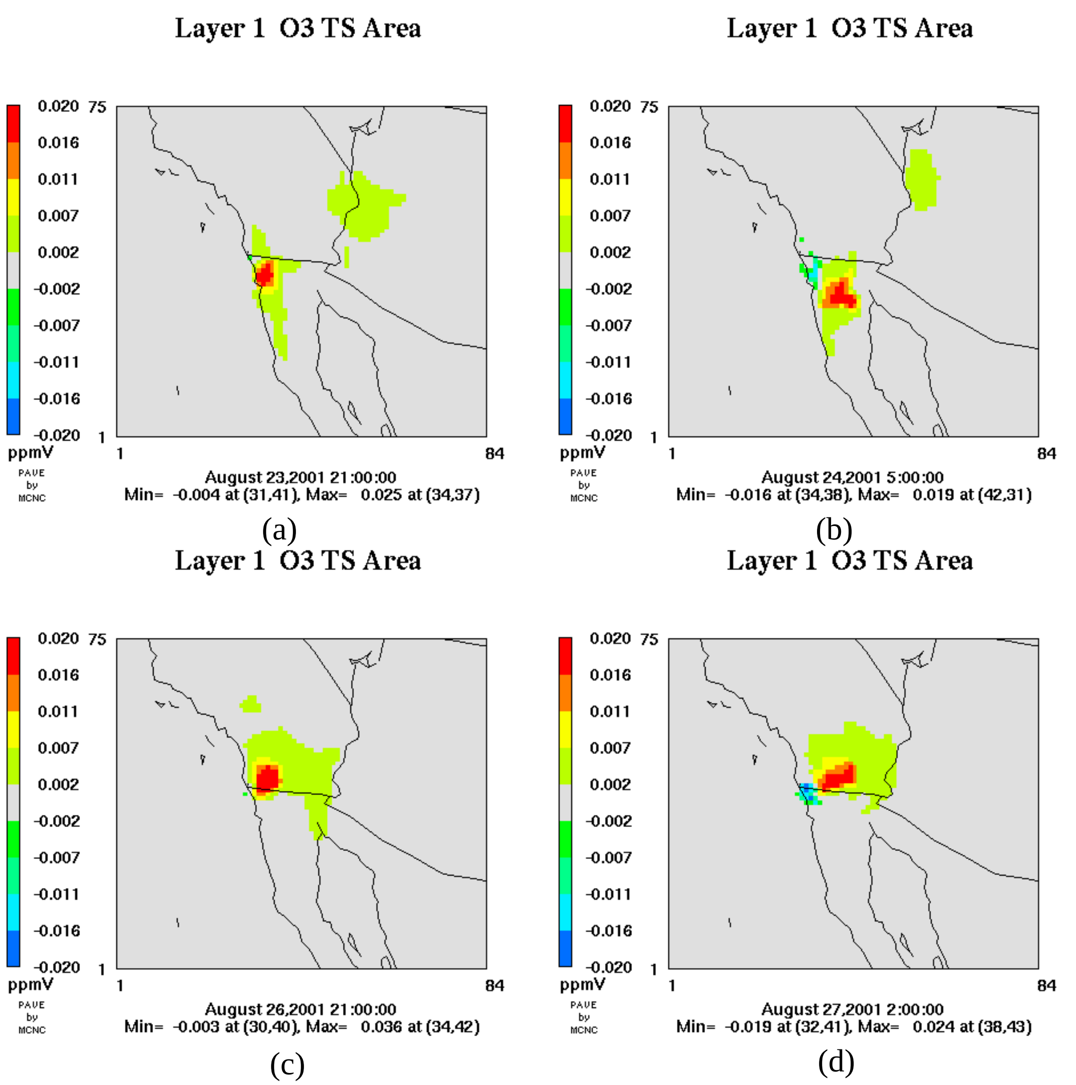
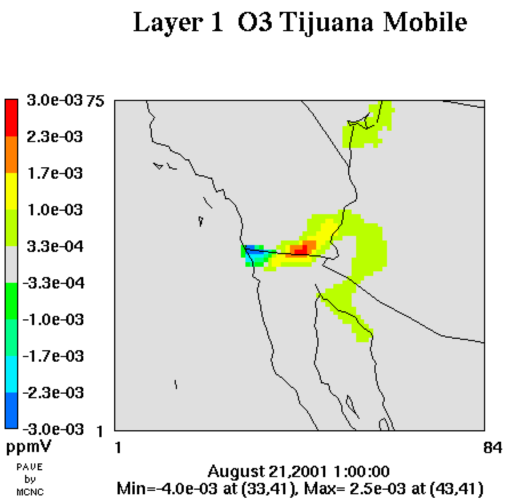
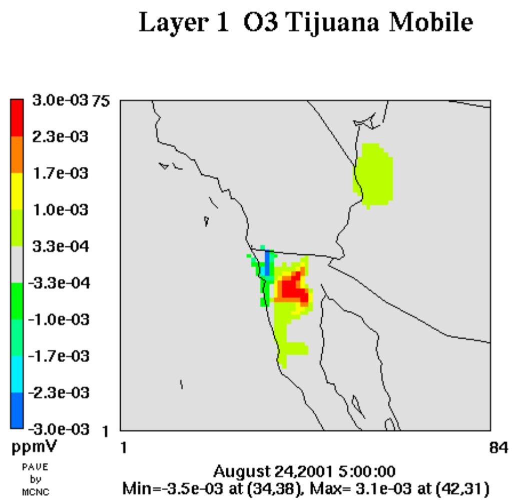


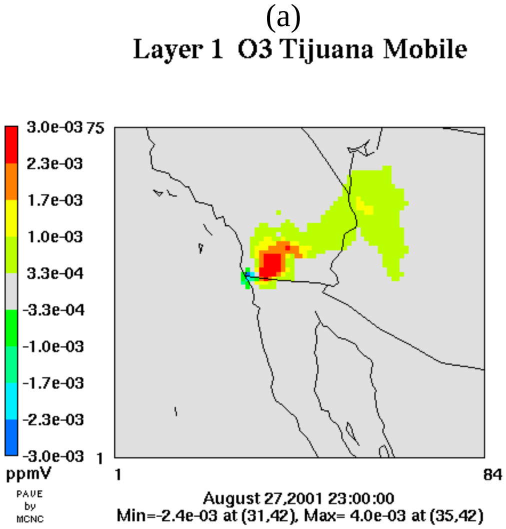
Figure 3.13 (a) (b) O_3 plumes emerging from Tijuana area sources transported towards inner Baja California, (c) Plumes emerging from Tijuana-San Diego reaching the Mexicali-Calexico region



(a)

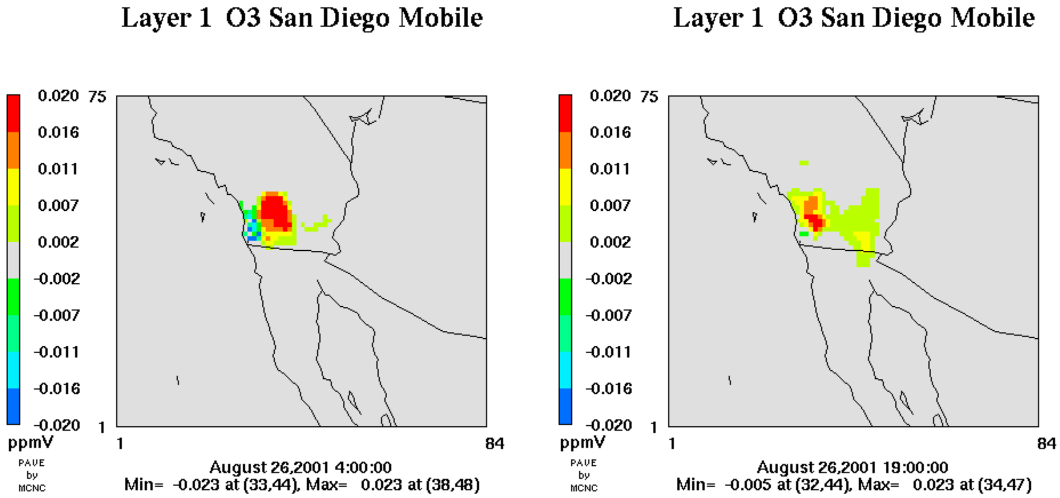


(b)



(c)

Figure 3.14 (a) O_3 plumes from Tijuana mobile sources impacting Calexico-Mexicali region ranging up to 3 ppbv, (b) O_3 plumes moving towards inner parts of Baja California, (c) O_3 plumes being carried northeast towards Arizona



(a) (b)

Figure 3.15 (a) Mobile sources in San Diego initiate the formation of up to 26 ppbv of O_3 around the region affecting neighboring state parks, (b) O_3 plumes being transported towards Calexico-Mexicali

3.3.4 January 2002 Episode

<u>3.3.4.1 Base Case</u>

As PM concentrations are a major concern during the winter season, we limit our discussion for the January 2002 episode predominantly to $PM_{2.5}$ dynamics across the region. The 24 hr average national standard for $PM_{2.5}$ is 35 µg m^{-3}. A peak of 188 µg m^{-3} is simulated on January 12, 2002 (18:00 hrs UTC) near Los Angeles. The movement of $PM_{2.5}$ plumes from Los Angeles, Las Vegas, San Diego-Tijuana and Mexicali-Calexico is represented in Figure 3.16. Plumes from San Diego-Tijuana, LA and Las Vegas unite and move towards the Mexicali-Calexico region with impacts of 10-35 µg m^{-3}. This transport along with MC emissions is carried further southeast inside Mexico. MC shows peak $PM_{2.5}$ concentration of 50 µg m^{-3}. Primary organic mass is the main contributor in Los Angeles contributing to a peak of 98 µg m^{-3}. The maximum contribution from primary organic matter in MC is 10 µg m^{-3}. Peak soil dust concentrations of 40 µg m^{-3} are found in Pheonix and Las Vegas areas during the winter episode. The soil dust contributions from LA, TS and MC range between 5-25 μg m^{-3} (Figure 3.17).

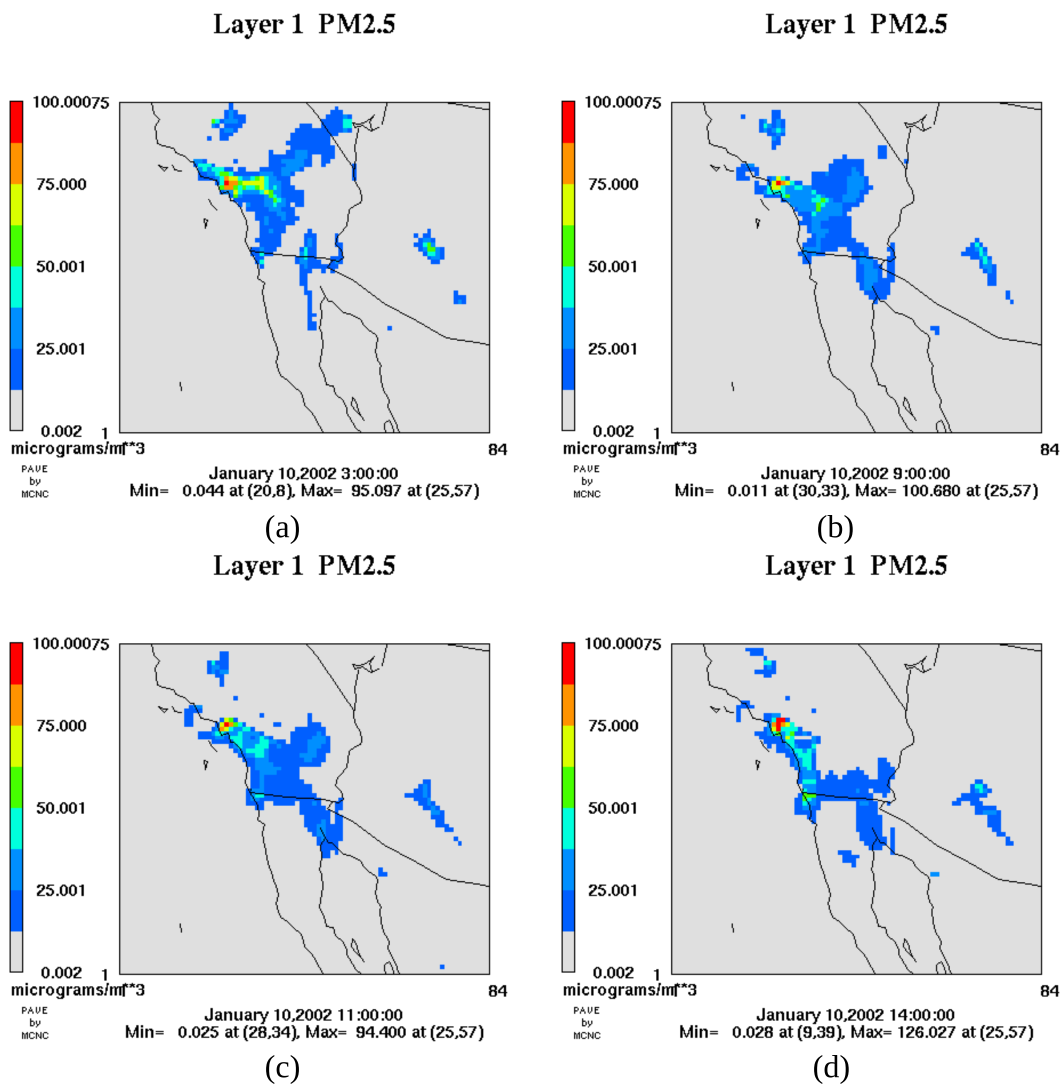


Figure 3.16 (a) (b) (c) $PM_{2.5}$ plumes from Los Angeles, Las Vegas, Tijuana-San Diego moving southeasterly towards Mexicali-Calexico during January 2002 Episode, (d) $PM_{2.5}$ impacts seen all across the border region between California and Baja California.

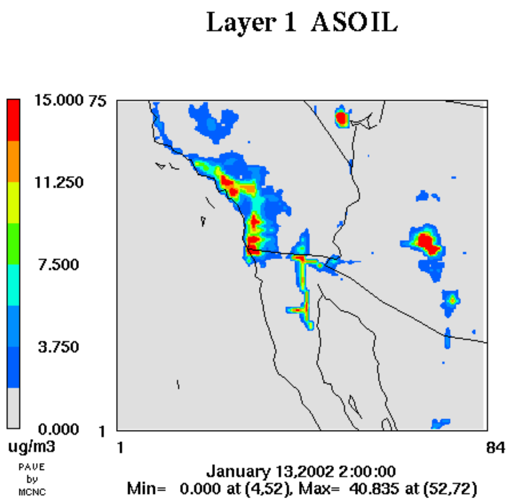
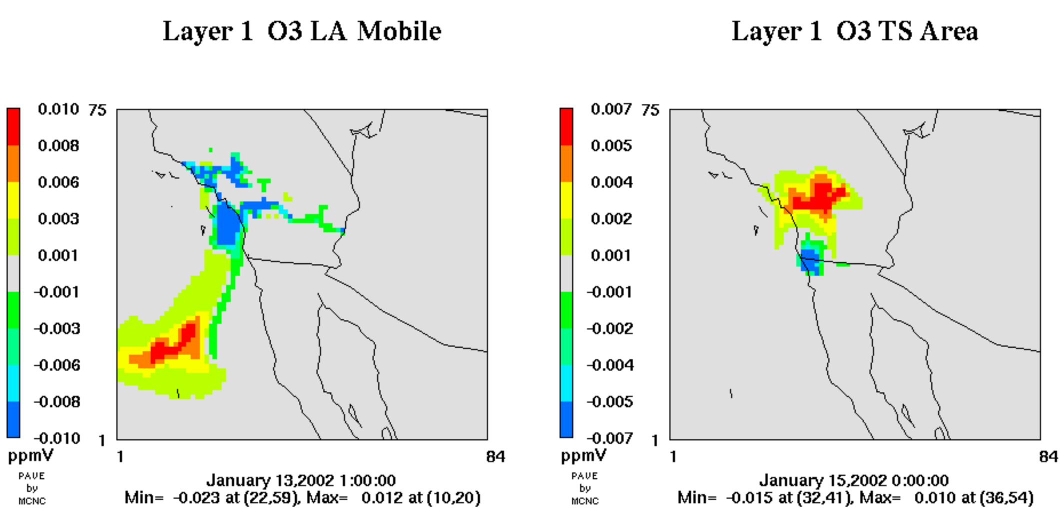


Figure 3.17 Soil dust contribution in Los Angeles, Tijuana-San Diego and Mexicali-Calexico

3.3.4.2 Source Contribution during January 2002 Episode

Contributions to O_3 from various sources in the region were simulated for the winter episode. Impact of LA mobile sources of up to 14 ppbv was seen over the Pacific Ocean. Plumes were also observed along the coast from Los Angeles to San Diego representing the major travel road route (Figure 3.18a). MC area sources had simulated impacts of up to 6 ppbv over the southern regions of Baja California.



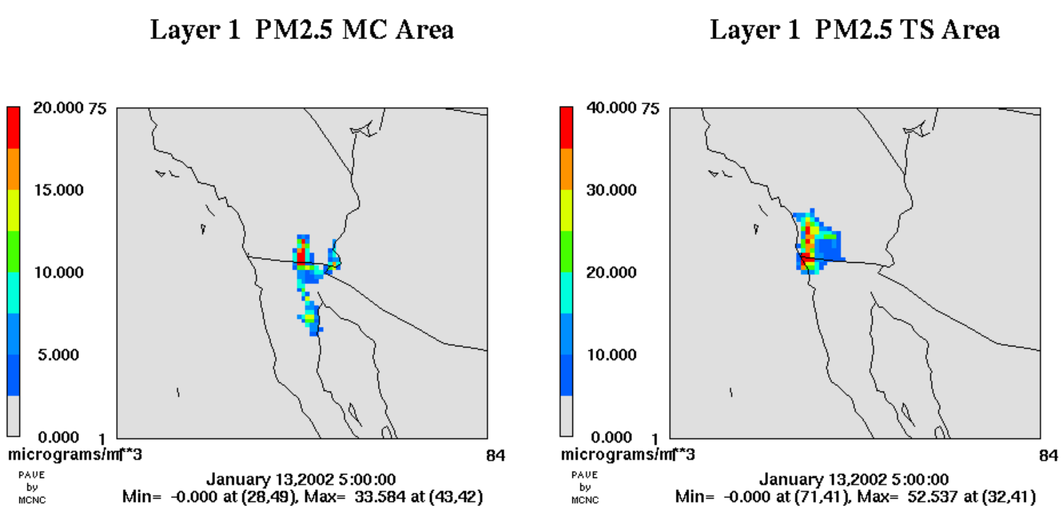
(a) (b)

Figure 3.18 (a) O_3 plumes formed from LA mobile sources moving towards Pacific Ocean, (b) Peak impacts of O_3 formed from TS area sources seen over LA region

However, much of the time fresh NOx emissions led to decreases (negative sensitivities) over urban areas. Peak impacts of 11 ppbv of O_3 is simulated over the Los Angeles area during the winter episode which originate from TS area sources (Figure 3.18b).

Similar values as that in summer episode are simulated with peak impacts of up 2 ppbv O_3 on the Baja California region from Mexicali mobile emissions. Tijuana, San Diego and Calexico mobile sources contribute to less than 6 ppbv O_3 during the winter episode.

MC area sources contribute to a simulated $PM_{2.5}$ maximum of 34 µg m^{-3} (Figure 3.19a). The pattern is much localized. Primary $PM_{2.5}$ emissions from MC mobile sources contribute negligibly with peak contributions of 0.5 µg m^{-3}. Secondary formation mechanisms form important sources of $PM_{2.5}$. MC point sources, primarily present in Mexicali contribute to a maximum of 12 µg m^{-3} over the border region. Area sources in TS have very large contributions, ranging up to 52 µg m^{-3} (Figure 3.19b). TS mobile sources contributed to less than 3 µg m^{-3} of primary $PM_{2.5}$. Point sources in San Diego contributed to a maximum 13 µg m^{-3} of primary PM2.5 in the region.



(a) (b)

Figure 3.19 (a) Peak contribution of $PM_{2.5}$ from MC primary $PM_{2.5}$ area source during January 2002, (b) Peak impacts from $PM_{2.5}$ TS primary sources during January 2002

3.4 Summary

O_3 and $PM_{2.5}$ concentration dynamics during the pollution episodes of July 2001, August 2001, and January 2002 are analyzed for the border regions of Mexicali-Calexico and Tijuana-San Diego. These pollutant dynamics are also then associated with the emissions and transport of pollutants from Los Angeles and its neighboring areas. Source contributions from area, point and mobile sources in these regions is also analyzed for the summer and winter episodes. O_3 and $PM_{2.5}$ concentrations in the domain are the highest in the LA area. During the summer episode, O_3 plumes originating from Tijuana-San Diego are transported eastwards along the border region towards Mexicali-Calexico. O_3 plumes generated from precursors emitted by LA mobile sources are transported towards Mexicali-Calexico and add up to 10 ppbv in the MC region. Due to the north easterly direction of the winds, O_3 plumes also reach the Grand Canyon National Park area with impacts ranging up to 10 ppbv. Though, mobile sources are of concern in the MC area, O_3 impacts from the precursors in the region itself were virtually negligible from the simulated results. Area sources in MC contribute to a maximum of 8 ppbv of O_3 during the summer episode. O_3 plumes reach the border regions of California-Arizona and O_3 concentrations up to 4 ppbv in the Grand Canyon area can be attributed to area sources in the MC region. O_3 plumes from Tijuana are transported in the southeast direction into inner Baja California and impact up to 20 ppbv of O_3. Plumes up to 3 ppbv of O_3 reach Mexicali-Calexico from Tijuana mobile sources. Mobile sources from San Diego have a contribution of up to 26 ppbv of O_3 in the region itself, and also over the park areas such as Anza Borrego Desert State Park located southeast of San Diego. Contribution of up to 11 ppbv of O_3 in Calexico-Mexicali can be attributed to the high density of vehicles in and around the San Diego region. About 50% of the $PM_{2.5}$ concentration in MC can be attributed directly to the area sources in August 2001.

During the winter episode, the winds being southeasterly (towards southeast) plumes from San Diego-Tijuana, LA and Las Vegas unite and move towards the Mexicali-Calexico region with impacts of 10-35 μg m^{-3}. The soil dust contribution from LA, TS and MC ranges between 5-25 μg m^{-3}. MC area sources contribute a maximum of 34 μg m^{-3} $PM_{2.5}$. Area sources in TS have a very large contribution ranging up to 52 μg m^{-3} over the surrounding regions.

3.5 Acknowledgements

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CHAPTER 4

AIR POLLUTION IMPACTS FROM CROSS BORDER POWER TRANSMISSION FROM TWO NATURAL GAS POWER PLANTS LOCATED IN THE UNITED STATES- MEXICO BORDER REGION

4.1 Introduction

Future energy requirement studies have been able to project pollutant emissions from the growing number of power plants in the border regions [1]. However, the transport of pollutants from individual power plants and their impacts on either sides of the border has not been conducted. With the commissioning of new power plants in the border regions of California and Baja California, concerns have increased over the impact of these power plant emissions over both sides of the border. These plants supply energy to the growing needs in the border region and parts of California.

Two such natural gas-fired, combined-cycle power plants, La Rosarita Power Complex (LRPC) and Termoeléctrica de Mexicali (TDM) (henceforth addressed as Intergen and Sempra, respectively, in reference to their operators) located in Mexicali (Baja California), 7 miles away from the US-Mexico border are studied (Figure 4.1). La Rosarita Power Complex (LRPC) has two separate units. LR-1 (unit 1) is partly owned and operated Energia Azteca X S. de R.L. de C.V. (EAX), a subsidiary of InterGen power company has a capacity of 750 MW. 660 MW of this are contracted by CFE (Comisión Federal de Electricidad, the government enterprise tasked with the ownership and operation of the public electric system infrastructure) under a power purchase agreement and 90 MW are exported to California. LR-2 (unit 2) owned by Energia de Baja California (EBC) S. de R.L. de C.V. has a capacity of 310 MW exclusively dedicated to export. Termoeléctrica de Mexicali (TDM), a Sempra subsidiary owns and operates the 650 MW combined cycle generating facility located very close to Intergen.

The power plant produces electricity exclusively for export to the United States, transmitted over a transmission line not connected to the CFE transmission system.

Figure 4.1 Location of Intergen and Sempra Power Plants

Air quality modeling simulations using CMAQ/DDM3D-PM [2] were performed to estimate the impact of Intergen and Sempra emissions on O_3 and $PM_{2.5}$ concentration levels in the region during a representative summer pollution episode (August 2001), and a winter pollution episode (January 2002). Discussion of the representative episodes was presented in Chapter 2.

PM from unpaved roads are a primary concern, so additional results are analyzed on a scenario in which all the roads in Mexicali are paved. A proportionate analysis from the above Mexicali paving scenario is also extended in order to simulate the effects of offsetting $PM_{2.5}$ emissions from the two power plants by paving equivalent lengths of roads in Mexicali.

4.2 Method

4.2.1 CMAQ/DDM

Isolating effects of an individual emissions source on secondary air pollutants such as ozone and some components of particulate matter must account for complex non-linear processes, be sensitive to small emissions perturbations, and account for impacts that may occur hundreds of kilometers away. The ability to evaluate these impacts is becoming increasingly important for efficient air quality management [3] . However, isolating the impacts of an individual source on secondary pollutants such as ozone and some components of particulate matter (PM) must incorporate non-linear processes and be sensitive to small emissions perturbations. Additionally, because ozone is a regional pollutant, potential impacts over a large spatial domain must be considered [4]. While the Brute-Force method is useful for large scale perturbations, numerical errors may exceed the perturbation of the parameter if the perturbation is small, such as those from even a large single source [5]. The Brute Force method (In this case, the difference between the pollutant concentrations with power plants, and pollutant concentrations without power plants (Base case) introduces additional uncertainties. Natural gas power plants are very clean as compared to their coal fired counterparts. Therefore the differences in pollutant concentrations between base case and base case with power plants are very small. They tend to be many times smaller than the model “numerical noises”. Hence, using the Decoupled Direct Method (DDM) which calculates the derivative of a pollutant response to a perturbation is very useful. This derivative can be linearly extrapolated to estimate a resulting pollutant concentration.

The 12 km domain as described in Chapter 3 is used for air quality simulations. To understand the impacts of emissions from sources on species concentrations, the first order semi-normalized sensitivities are obtained using CMAQv4.5 /DDM-PM [2, 6-8]. Sensitivity of C_i to emission perturbations can be stated as follows:

$$S_{i,j}^{(1)} = \frac{\partial C_i(x,t)}{\partial \mathrm{E}_i} \tag{4.1}$$

where E_j is the relative emission perturbation.

4.2.2 Power Plant Emissions

Emissions for base case results (i.e., without power plants) are obtained as discussed in Chapter 3, Section 3.2.2. These emissions are then added to Intergen and Sempra emissions separately. These become the emission inputs to CMAQv4.5 /DDM-PM model. Emissions modeling using SMOKE and Meteorological modeling using MM5 for these episodes are already discussed in Chapter 2 and 3.

Three different power plant emission scenarios are used (personal communication with Dr. Allen Blackman, RFF). Scenario 1 (DOE): Emission values for Intergen and Sempra plants as given by the Environmental Assessment Report prepared for the Government Accountability Office [9]; Scenario 2 (TPT): Emission values obtained from the power plants, as tested by a third party. The tests were held between September 20 and September 28, 2004 for Intergen , and during June 4-6, 2003 and July 8-9, 2003 for Sempra by Air Hygeine International, Inc [9]; Scenario 3 (CAREG): Emission values if both Intergen and Sempra plants were located in California and thus following California emission standards (Table 4.1). Sempra plant had emissions which were already within California emission standards, however, emissions of carbon monoxide (CO) and nitrogen dioxide (NO_2) standards got tightened for Intergen in the CAREG scenario as compared to third party testing. Third party testing was conducted for PM_{10}, VOC, NH_3

and NO_2 emissions. Emission values for Intergen were combined from both EAX and EBC units.

Table 4.1 Emissions from Intergen and Sempra Plants for DOE, TPT, and CAREG Scenarios. Units are in short tons per year.

	DOE		TPT		CAREG	
Pollutant	**Intergen**	**Sempra**	**Intergen**	**Sempra**	**Intergen**	**Sempra**
NOx	423	187.32	302	155.95	228.83	155.95
PM10	957	255.8	130.02	126.81	130.02	126.81
PM2.5	916	237	NM*	NM	NM	NM
CO	2908.32	181	63.42	0	0	0
NH3	370	276	58.78	11.24	58.78	11.24
VOC	685	384	8.19	undetected**	8.19	undetected
SO2	19.18	10.752	NM	NM	NM	NM

*NM- not measured
**undetected- smaller than instrument measurement limits

4.3 Results and Discussion

4.3.1 Impact from Intergen Plant

Peak impact of 1 ppbv of O_3 is observed in Mexicali during the August 2001 episode from Intergen. Though the impacts are small, transport of pollutants occurs away from the border region. The wind direction being predominantly northeast during the summer episode, O_3 plumes from the Intergen plant are seen to be effecting the Calexico region, as well as, the border region between California and Arizona (Figure 4.2a, c, d). O_3 impacts up to 6.2×10^{-1} ppbv move into Arizona (Figure 4.2e). Grand Canyon National park area located east of Las Vegas is also hit by the O_3 plume adding an additional up to 5.6×10^{-2} ppbv (Figure 4.2f). Plumes are also seen to move inwards towards Sonora, Mexico following the wind path. Ozone impacts during winter are negligible with peak impacts reaching 1×10^{-3} ppbv.

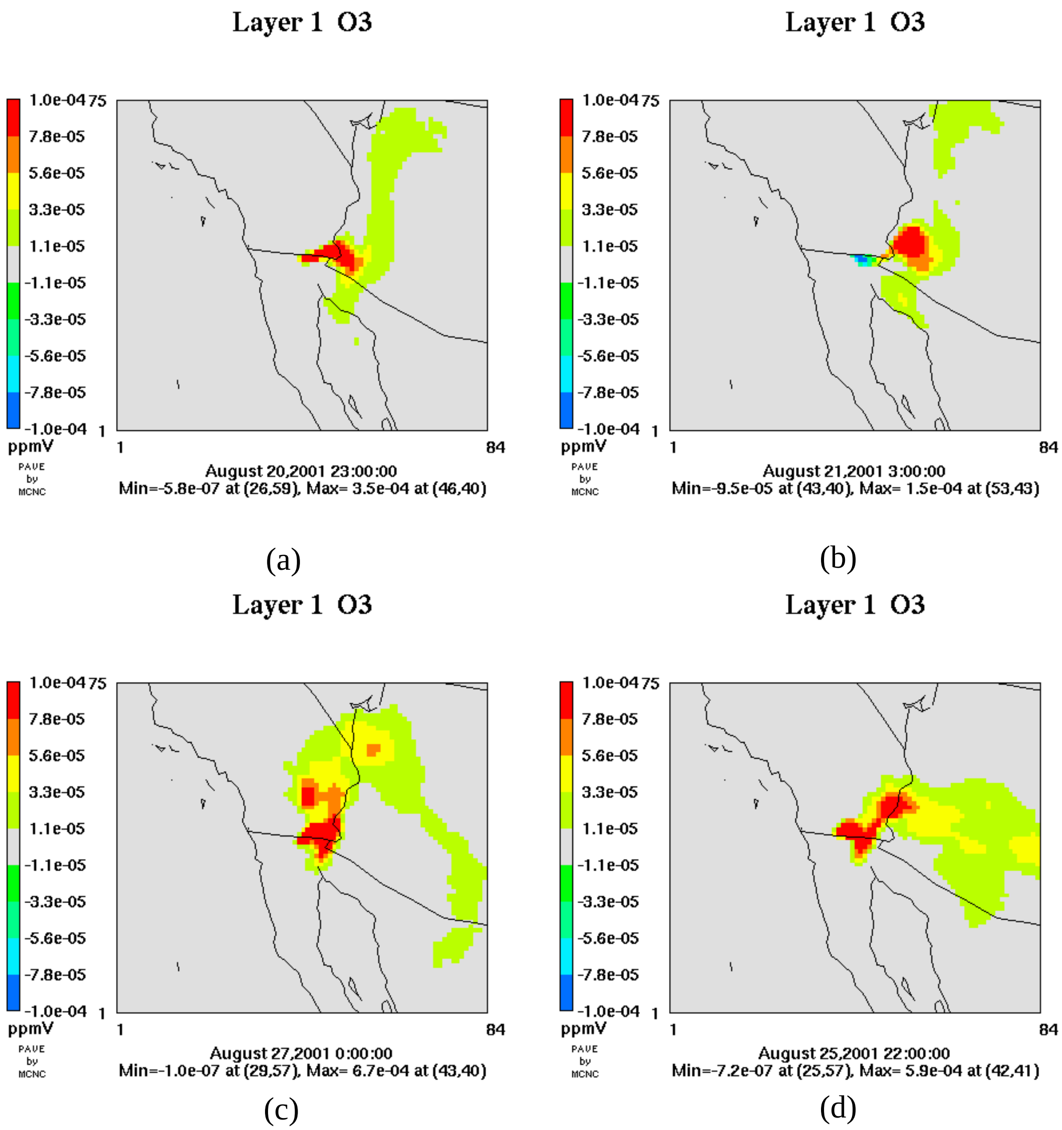
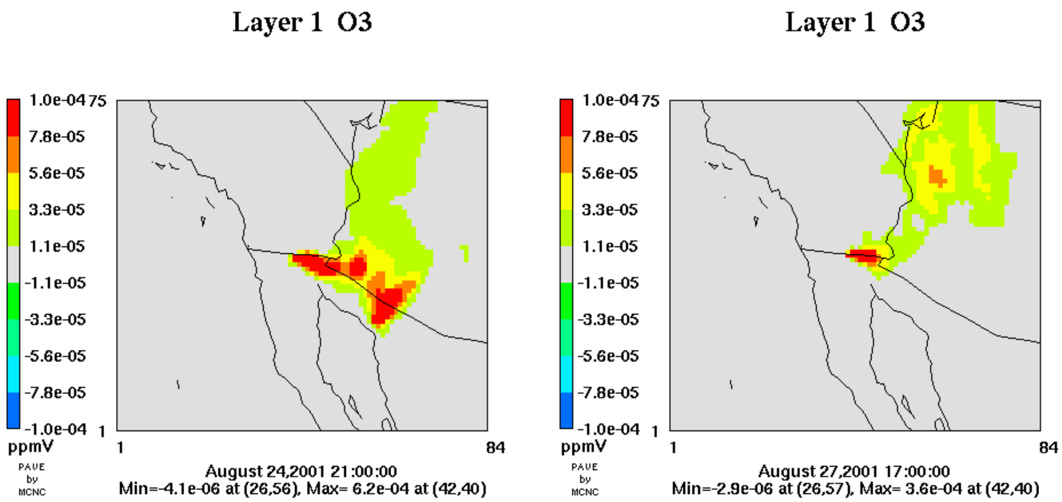


Figure 4.2 (a) (b) (c) O_3 Plumes from Intergen Plant being transported to the Border Region between California and Arizona, (d) O_3 Plumes impacting Arizona and parts of Sonora, Mexico



(e) (f)

Figure 4.2 continued (e) O_3 Plumes impacting Arizona and parts of Sonora, Mexico, (f) O_3 Plume transported towards Grand Canyon National Park

Maximum impacts of 2.2 µg m^{-3} $PM_{2.5}$ is seen in the Mexicali-Calexico during the winter episode. Since the winds are southwards during winter, the pollutants are transported inwards to other parts of Baja California (Figure 4.3a, b, c). The southerly moving $PM_{2.5}$ plumes has a maximum impact of 1.2 µg m^{-3} on the southern regions of Baja California. Plumes ranging up to 3.3×10^{-2} µg m^{-3} are transported towards Nevada (Figure 4.3d).

Since the pollutant impacts are very small, the emission impacts over the region can be considered to be linear over the modeling domain. Emission values for scenarios 2 (TPT), and 3 (CAREG) are proportionately smaller than the DOE emissions (Table 4.1). Therefore, the concentration impacts are also linear with respect to emissions. Considering that these impacts are very small as compared to the DOE case, we limit our discussion to the DOE scenario in this thesis.

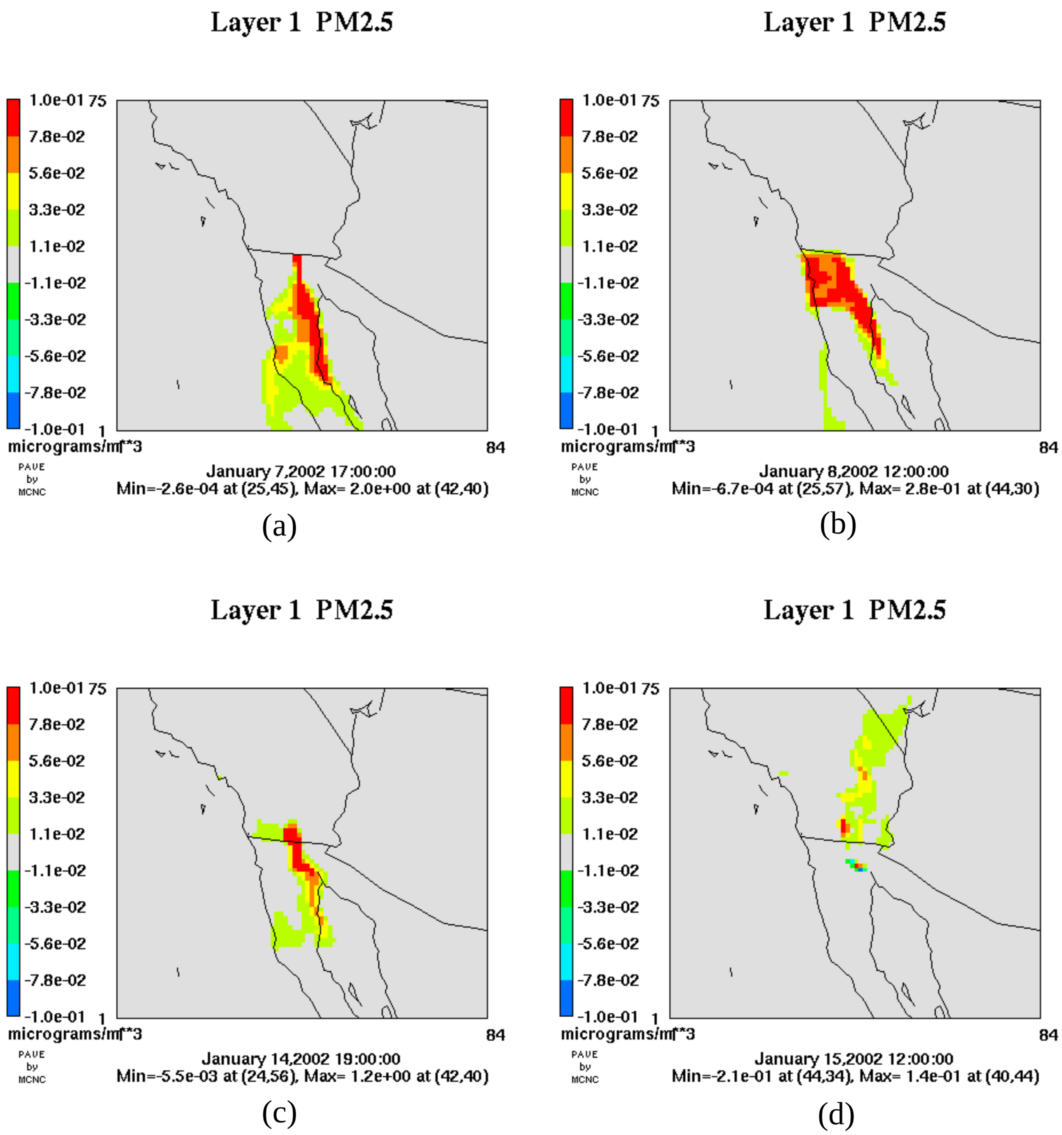


Figure 4.3 (a) (b) (c) $PM_{2.5}$ plumes being transported to regions of Southern Baja California, (d) PM2.5 plumes from Intergen transported to Nevada

4.3.2 Impact from Sempra Plant

Energy supply capacity of Sempra is 61.3% that of Intergen. The maximum impact from Sempra for O_3 is 4×10^{-1} ppbv over the Mexicali-Calexico region. Plumes upto 3.4e-4 ppmv are seen transported into California and Arizona (Figure 4.4a, b). Similar to the Intergen plumes, Sempra plumes are transported towards the Grand Canyon National Park area ranging upto 1.6×10^{-2} ppbv (Figure 4.4c, d). During the winter episode, peak impact of 0.57 µg m^{-3} is simulated over Mexicali. $PM_{2.5}$ plumes are transported to other regions of Baja California, including Tijuana (Figure 4.5).

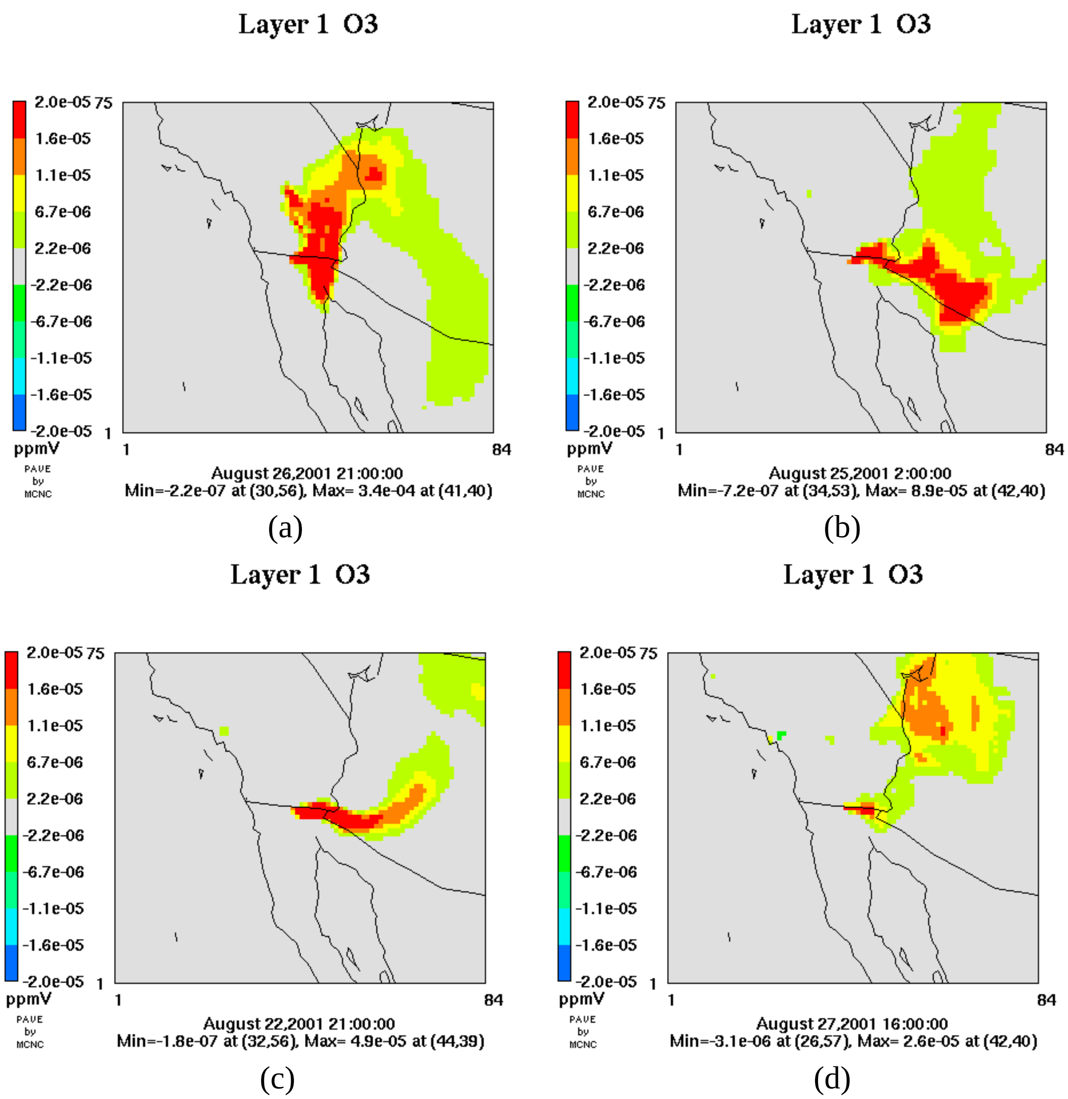


Figure 4.4 (a) (b) O_3 plume from Sempra plant transported to California and Arizona, (c) (d) O_3 plume from Sempra reaching Grand Canyon National Park area

4.3.3 Paving 100% of the Roads in Mexicali

As discussed in Chapter 3, PM emissions from unpaved roads in Mexicali contribute to the air quality deterioration over the border region. According to the Border Environment Cooperation Commission [10], approximately 63% of the roads in Mexicali were paved by 2002. Projects such as PIPCA (Air Quality Improvement and Street Paving Program) initiated by the State of Baja California have been working towards paving roads. According to the 5 year plan proposed in 2003, by the year 2007 almost 80% of the roads in Mexicali were to be paved. For our simulations, we have assumed that 63% of the roads were paved in 2001, and a future case scenario of 100% road paving is compared with it. No distinction is made between urban, sub-urban and rural roads. PM_{10} emissions from NEI 2001 emissions inventory gives values of 4050 short tons year^{-1} from paved roads and 66640 short tons year^{-1} from unpaved roads in Mexicali. $PM_{2.5}$ emissions were 683 short tons year^{-1} and 14130 short tons year^{-1} from paved and unpaved roads respectively. Assuming 100% of the roads in Mexicali were to be paved in future, the emissions from paved roads becomes 6425 short tons year^{-1} of PM_{10} and 1085 short tons year^{-1} of $PM_{2.5}$ emissions by proportionality.

In order to understand the overall impact of this change over the region CMAQv4.5 was applied using a Brute Force approach to simulate $PM_{2.5}$ results (i.e., Base Case minus 100% Mexicali paved scenario). A maximum $PM_{2.5}$ concentration reductions of up to 10 μg m^{-3} on the Mexicali region is simulated, while the peak $PM_{2.5}$ concentration reductions in Calexico is around 6 μg m^{-3} during the summer episode (Figure 4.6a). During the winter episode, the peak benefit from paving roads is 13 μg m^{-3} of $PM_{2.5}$ in Mexicali, and up to 8 μg m^{-3} in the Calexico region (Figure 4.6b, c). Benefits of up to 0.5 μg m^{-3} are simulated in the lower regions of Baja California.

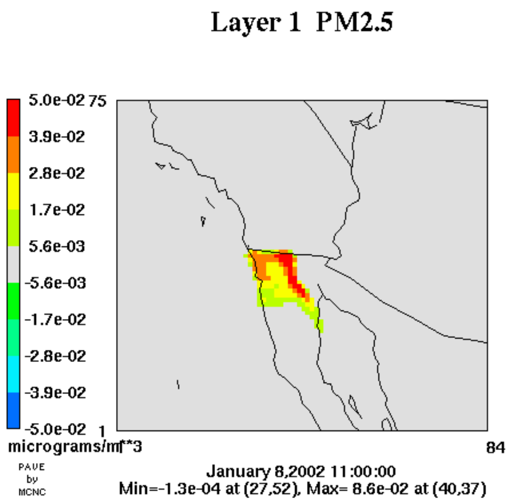


Figure 4.5 $PM_{2.5}$ impacts from Sempra Plant during the winter episode

An additional scenario was developed by RFF to offset $PM_{2.5}$ emissions from the two power plants by paving equivalent amount of unpaved roads. As a result, 2.16 miles of unpaved road were to be paved, and benefits were reduction in PM_{10} emissions by 243 short tons year^{-1}. The air quality benefits from paving 2.16 miles were simulated to be very small on a 12 km grid level domain.

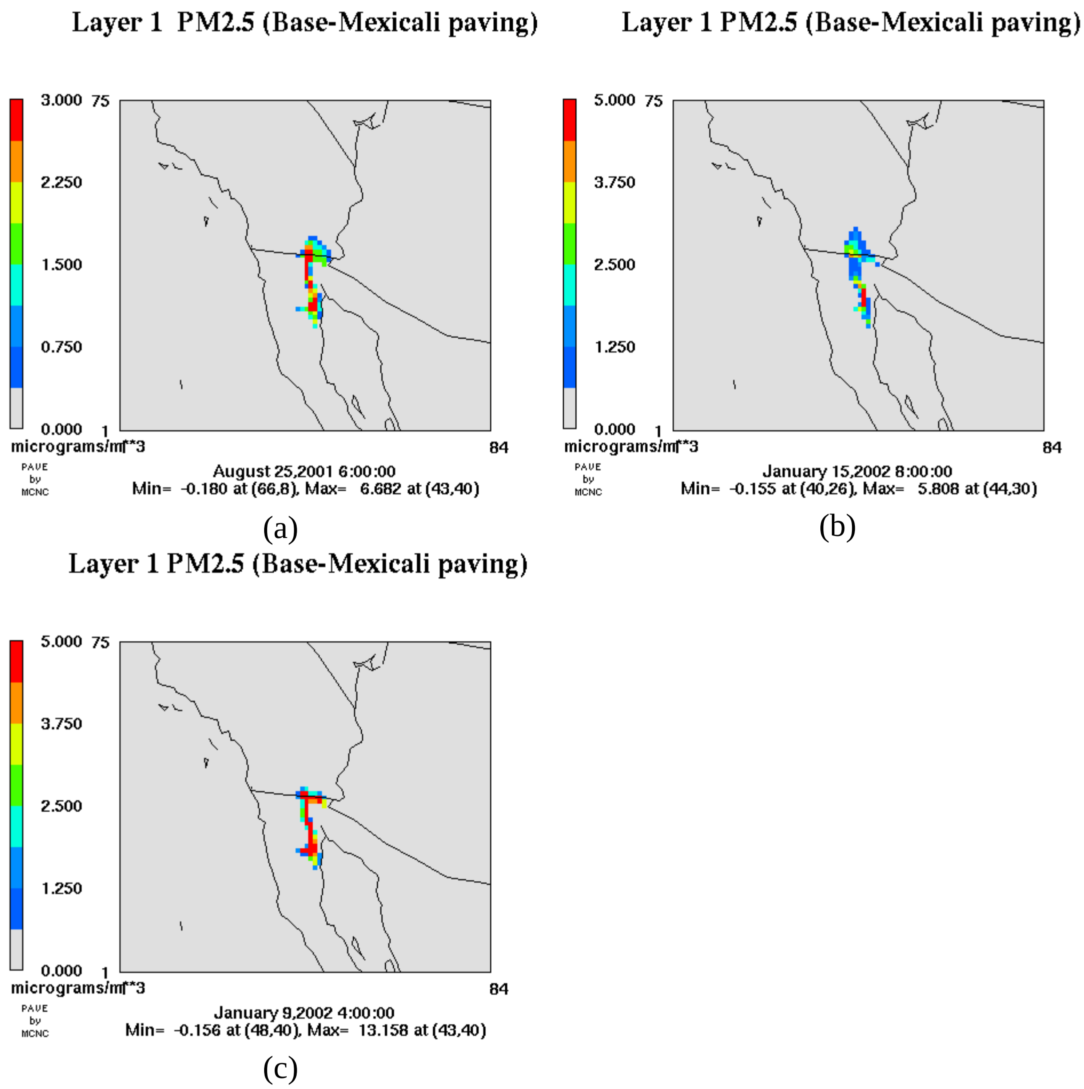


Figure 4.6 $PM_{2.5}$ impacts by paving 100% of Mexicali roads during (a) Summer episode, (b) Winter episode, (c) Peak impact of $PM_{2.5}$ concentrations simulated during winter episode.

4.4 Summary

Simulated peak O_3 impacts from Intergen during the summer episode of August 2001 are up to 1 ppbv in Mexicali, while that from Sempra are 0.4 ppbv over the Mexicali-Calexico region. The predominant wind pattern is northeasterly during Summer 2001 in the border region, hence O_3 plumes get transported to California, Arizona, and Sonora in Mexico. O_3 impacts up to 5.6×10^{-2} ppbv from Intergen reach the Grand Canyon

National Park area. $PM_{2.5}$ impacts during the winter episode of January 2002 are predominantly over Tijuana and southern regions of Baja California. Peak $PM_{2.5}$ impacts of up to 2.2 μg m^{-3} from Intergen and 0.57 μg m^{-3} from Sempra are seen over the Mexicali-Calexico region.

4.5 Acknowledgement

Author would like to thank the Latin American Scholarship Program of American Universities (LASPAU) funded Border Ozone Reduction and Air Quality Improvement Program for supporting this work. Author would also like to acknowledge Dr. Allen Blackman, and Zhuxuan You at Resources for Future (RFF), Washington DC for their support and guidance at all times during the project.

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CHAPTER 5

CONCLUSIONS

O_3 and $PM_{2.5}$ concentration dynamics during the pollution episodes of July 2001, August 2001, and January 2002 are analyzed for the border regions of Mexicali-Calexico and Tijuana-San Diego. These pollutant dynamics are also then associated with emissions and transport of pollutants from Los Angeles and its neighboring areas. Source contributions from area, point and mobile sources in these regions are also analyzed for the summer and winter episodes. O_3 and $PM_{2.5}$ concentrations in the domain are the highest in LA area. During the summer episode, O_3 plumes originating from Tijuana-San Diego are transported eastwards along the border region towards Mexicali-Calexico. O_3 plumes generated from the O_3 precursors emitted by LA mobile sources are transported towards Mexicali-Calexico increasing levels by up to 10 ppbv in the MC region. O_3 plumes also reach Grand Canyon National Park area elevating levels by up to 10 ppbv. Mobile sources are a concern in the MC area, though O_3 impacts from the precursors in the region itself were small from the simulated results. Area sources in MC contribute to a maximum of 8 ppbv of O_3 during the summer episode. O_3 plumes from MC reaches the border regions of California-Arizona elevating levels up to 4 ppbv in the Grand Canyon area from area sources in the MC region. O_3 plumes from Tijuana are transported in the southeast direction into the inner Baja California area with impacts up to 20 ppbv of O_3. Impacts of up to 3 ppbv reach Mexicali-Calexico from Tijuana mobile sources. Mobile sources from San Diego contribute up to 26 ppbv of O_3 on the region itself, and also over Class I areas such as Anza Borrego Desert State Park located southeast of San Diego. Contribution of up to 11 ppbv of O_3 in Calexico-Mexicali can be attributed to the high density of vehicles in and around the San Diego region. About 50% of the $PM_{2.5}$ concentration in MC can be attributed directly to the area sources in August 2001.

During the winter episode, the winds being southeasterly (towards southeast), plumes from San Diego-Tijuana, LA and Las Vegas unite and move towards the Mexicali-Calexico region increasing $PM_{2.5}$ by 10-35 µg m^{-3}. Soil dust contributions from LA, TS and MC range between 5-25 µg m^{-3}. MC area sources contribute a maximum of 34 µg m^{-3} $PM_{2.5}$ in the region. Area sources in TS have a very large contribution ranging up to 52 µg m^{-3} over the surrounding regions.

Simulated peak O_3 impacts from Intergen during the summer episode of August 2001 are up to 1 ppbv in Mexicali, while that from Sempra are 0.4 ppbv over the Mexicali-Calexico region. The predominant wind pattern is northeasterly during Summer 2001 in the border region, hence O_3 plumes get transported to California, Arizona, and Sonora in Mexico. O_3 impacts up to 5.6×10^{-2} ppbv from Intergen reach the Grand Canyon National Park area. $PM_{2.5}$ impacts during the winter episode of January 2002 are predominantly over Tijuana and southern regions of Baja California. Peak $PM_{2.5}$ impacts of up to 2.2 µg m^{-3} from Intergen and 0.57 µg m^{-3} from Sempra are seen over the Mexicali-Calexico region.

CHAPTER 6

FUTURE WORK

In the current work, Mexicali mobile emissions are treated as area sources, as VMT data was not available for the processing with Mobile 6 at the time of simulations. With the release of the latest Mexico Border States inventory in 2007 by USEPA, this shortcoming has been filled. Future simulations should be run with updated Mexico mobile inventory, and should be compared to the current case.

This work forms a platform in order to understand the pollutant dynamics of O_3 and $PM_{2.5}$ in the border areas of Tijuana-San Diego and Mexicali-Calexico. However, in order to regulate emissions from various sources, an analysis representing impacts from specific source categories should also be performed. Cross sensitivities i.e., impacts of precursors on pollutant concentrations in different regions should be performed in order to better quantify the role of emissions in one region on the pollutant concentrations of other.

APPENDIX A

REPRESENTATION OF THE TAF MODEL AND LOCATION OF REPRESENTATIVE MONITORING SITES

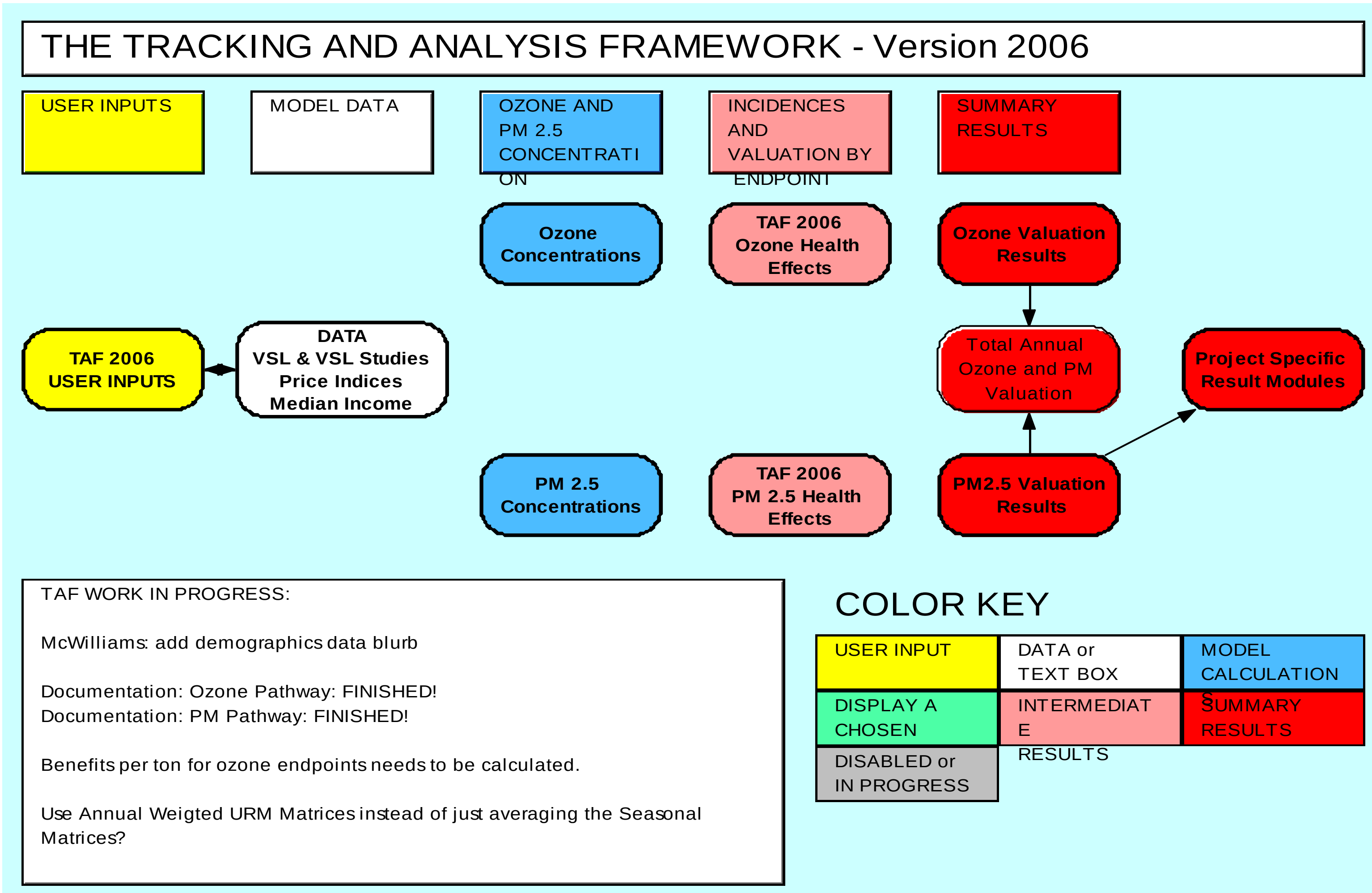
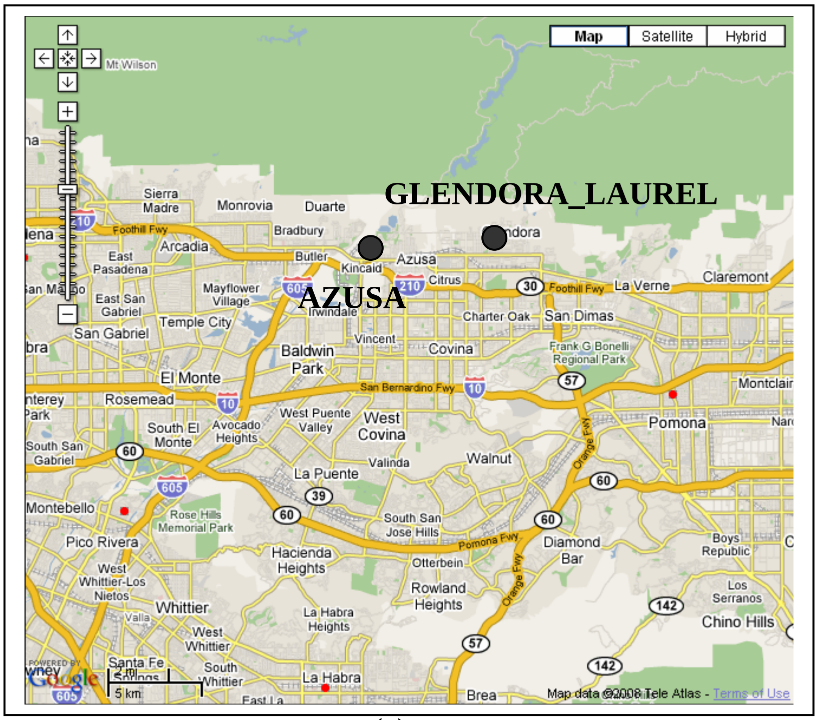
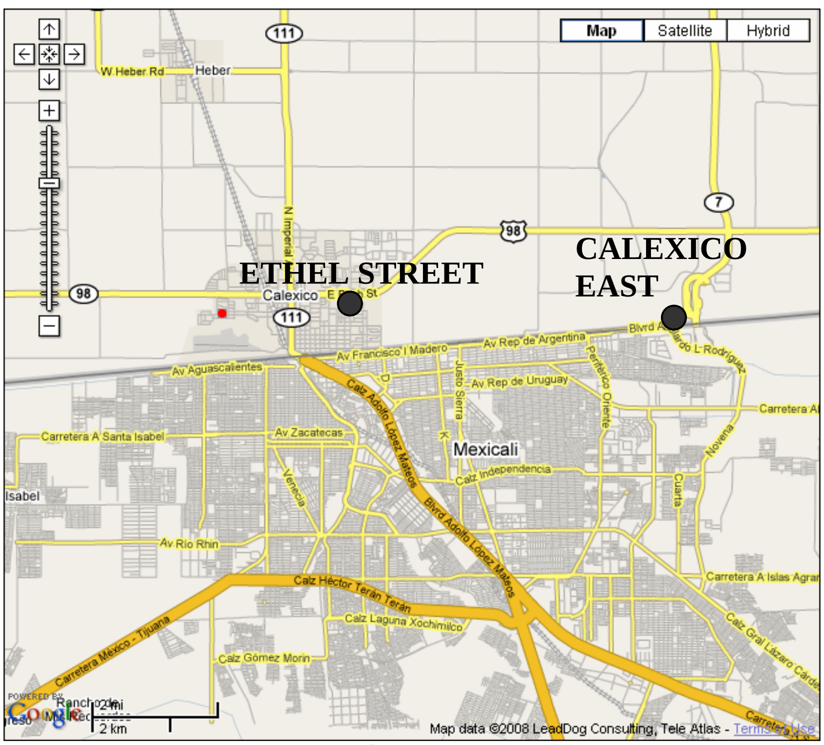


Figure A.1 Tracking and Analysis Framework Model



(a)



(b)

Figure A.2 Maps showing the location of representative monitoring sites in Los Angeles and Mexicali-Calexico Source: California Air Resources Board (http://www.arb.ca.gov/qaweb/mapdemo/map_module.php)